#### Directorate for Mathematical and Physical Sciences Advisory Committee Meeting Minutes April 22-23, 2004

Thursday, April 22, 2004 Morning Session

#### **Welcoming Comments**

Dr. Jeanne Pemberton, Chair of the Mathematical and Physical Sciences Advisory Committee (MPSAC), called the meeting to order at 8:10 AM. After welcoming the attendees, the Chair called on Dr. Michael Turner, the Assistant Director for the Directorate for Mathematical and Physical Sciences (MPS) to provide an update on National Science Foundation (NSF) and MPS activities. Attendees at the meeting are listed in Appendix I.

#### Discussion by Dr. Michael Turner, Assistant Director, MPS

Dr. Turner described the change in leadership at NSF that had taken place since the last meeting of the MPSAC. Dr. Rita Colwell had stepped down as NSF Director on February 20, 2004. She had accomplished many things for NSF, and during her tenure the budget of NSF had increased by approximately 70%. President Bush had named Dr. Arden L. Bement, Jr., Director of National Institute of Science and Technology, as Acting Director of NSF. Bement was very familiar with NSF. Turner noted that an Acting Director could only serve for a period of 210 days. Pemberton asked when this 210-day period would be over, and Turner responded that it would be in the third week of September 2004. In response to a question, Dr. Morris Aizenman, the MPS Senior Science Associate, noted that this period could not be renewed. Dr. Venkatesh Narayanamurti asked whether Bement could be named the permanent NSF Director, and Aizenman stated that it was his understanding that this was not possible. Turner commented that at a recent NSF budget hearing Senator Bond had asked Dr. John Marburger, Director of the Office of Science and Technology Policy (OSTP) and the Presidential Science Advisor about the fact that Bement was juggling responsibilities between NSF and NIST, and Marburger responded that an aggressive search for an NSF Director was underway, and that the President expected to make an announcement within a month. However, Turner noted, two months had passed since that discussion.

Turner commented that NSF's FY2004 budget, which was enacted in late January of 2004, is 5% greater than the FY 2003 budget. This number represents an average of the House and Senate appropriation recommendations for NSF, less an 0.59% rescission.

NSF's FY 2005 budget request, currently being considered by Congress, represents an increase of 3% over NSF's current FY 2004 budget. This should be compared to the FY 2005 budget requests for the National Institutes of Health (up 2.6%), the Department of Energy's Office of Science (down 1%) and the National Aeronautics and Space Administration's (NASA) Office of Space Sciences (up 1%). This is the first year in a long time that NSF's percentage increase request is higher than that of NIH and should be considered in the light of a very challenging fiscal environment.

Turner commented that NSF is beginning to prepare for its FY 2006 budget request to the Office of Management and Budget (OMB). The NSF Acting Director, the Deputy Director, and the Assistant Directors had held a retreat earlier this month to begin discussions of this activity. There was an MPS Senior Staff retreat in January 2004 to begin FY 2006 budget planning.

In discussing NSF funding, Turner stated that overall, NSF appropriated budgets were up approximately 68% since 1998, but even these budgets were falling increasingly below authorization levels in recent years.

With respect to the NSF FY 2005 budget request currently before Congress, NSF is requesting an increase, compared to FY 2004, of 4.4% in the Research and Related Activities (R&RA) account, of 36.7% in the Major Research Equipment and Facilities Construction account (MREFC), and an increase of 34.4% in the Salaries and Expenses (S&E) account. The increase in the S&E account is NSF's highest priority in the FY05 budget request.

S&E is a major issue for NSF since this is the funding of program officers and their travel, and current support is too small. NSF spends only 5% of its total budget on S&E and it is very difficult to operate on such a lean budget. Program officers are at the breaking point. Dr. Judith Sunley, Executive Officer of MPS, commented that the bulk of the S&E requested increase is for an upgrade of NSF computer systems and their security. She also noted that in FY 2003 Congress had authorized NSF hiring an additional 25 individuals but had not appropriated the necessary funds. In FY 2004 Congress authorized hiring an additional 25 staff, and appropriated the money for the both these and for those authorized the previous fiscal year. In FY 2005, NSF is requesting funds to hire an additional 25 personnel.

Turner discussed the funding requests for FY 2005 for each NSF Directorate and Office. He noted that requested increases are roughly the same (in terms of percent) for all Directorates. Requested increases were leveling off because of the national budget deficit.

# NSF Budget Request \$\$ in Millions

	FY2003 Actual	FY 2004 Enacted	FY 2005 Request	Change \$ 05/04	Change % 05/04
R&RA	\$4,054.43	\$4,251.36	\$4,452.31	\$200.95	4.7%
MREFC	179.03	154.97	213.27	58.30	36.7%
EHR	934.98	938.98	771.36	-167.62	-17.9%
S&E	189.42	218.70	294.00	75.30	34.4%
OIG	8.70	9.94	10.11	0.17	1.7%
NSB	2.88	3.88	3.95	0.07	1.8%
Total: NSF	\$5,369.34	\$5,577.83	\$5,745.00	\$167.17	3.0%

Dr. William Pulleyblank asked about the decrease in funding for the Education and Human Resources Directorate (EHR). Turner responded that this decrease was due to OMB's decision to transfer the Math and Science Partnerships (MSP) program to the Department of Education. The transfer of funds to the Department of Education also affected the Research and Related Activities (R&RA) account, since of the \$200,000,000 in the MSP program, \$120,000,000 was in the EHR Directorate, while \$80,000,000 was in the R&RA account. The Administration request to fund the MSP program within the Department of Education rather than at NSF was a contentious issue within Congress. Dr. John Huchra commented that Congress could move the program back to NSF. Turner said that Congress had not passed an NSF funding bill yet, and the situation with respect to MSP did not directly involve MPS.

Huchra asked about NSF funding that went into facilities oversight. Turner responded that NSF felt that each major facility should have a program officer spending full time overseeing the facility. He also noted that NSF had a full-time Deputy Director for Large Facilities Projects, but this was only one person.

Turner then discussed the MPS FY 2005 budget request. MPS is requesting an increase of 2.2% (\$24,000,000) compared to the current FY 2004 budget or. This requested increase is not spread evenly across the MPS divisions.

MPS Budget Request FY 2005							
	FY2003 Actual	FY 2004 Enacted	FY 2005 Request	Change \$ 05/04	Change % 05/04		
AST	\$187.07	\$196.55	\$204.35	\$7.80	4.0%		
СНЕ	181.61	185.22	188.91	3.69	2.0%		
DMR	241.39	250.89	253.18	2.29	0.9%		
DMS	178.79	200.41	202.25	1.84	0.9%		
РНҮ	224.50	227.67	235.76	8.09	3.6%		
OMA	27.34	30.77	31.05	0.28	0.9%		
Total: MPS	\$1,040.70	\$1,091.51	\$1,115.50	\$23.99	2.2%		

Of this increase, \$14,000,000 would go to NSF initiatives while approximately \$10,000,000 would go to core activities within MPS. The core increase was spread evenly across the divisions. Turner commented that MPS is heavily involved in two of the five NSF priorities – Mathematical Sciences and Nanotechnology. The Physics of the Universe initiative request would receive \$12,000,000 to be equally shared by the Divisions of Astronomical Sciences (AST) and Physics (PHY). A second MPS initiative, Physical Processes to Enable Life from Cells and Ecosystems, would receive \$2,000,000 and would be administered in the Chemistry Division. He noted that within the requested MPS budget, activities related to Cyberscience would receive \$32,000,000. There were funds for mid-scale instrumentation, and for the Rare Symmetry Violating Processes (RSVP) project. This latter project was to a new start.

Dr. Joseph Salah asked if there were new money for mid-scale instrumentation, and Turner stated that there were no new funds, and funding for mid-scale instrumentation came from within the MPS budget. Salah commented that the MPSAC had recommended that in the balance between grants and bigger projects mid-scale instrumentation should be a set-aside with a separate budget. Turner commented that it was not possible to get new money for mid-scale instrumentation, and that there is no sentiment for creating a new line the NSF budget. NSF senior management felt that mid-scale instrumentation belonged within the directorates, and should not be a cross-foundation activity.

Dr. Frances Hellman commented that the community was sensitive to the percentage of funds going to individual investigators. It was the impression within her community that this percentage had been dropping. Turner responded by noting that funding for individual investigators varies radically across MPS divisions. AST argues that their facilities are part of their core, and they have only 15% of their budget going to individuals. Within the Division of Physics this percentage is 50%. Dr. Tom Weber, Director of the Division of Materials Research (DMR) stated that within DMR individuals receive 52% of divisional funds, and this percentage had been constant over 15 years. He added that the National Academy of Engineering had stated that NSF was forcing people to work in groups, but this was an incorrect perception. Part of this misperception came from the

NSF nanoscale announcement, which only mentioned groups and center, but grants for "two or more investigators" have been around for years.

Turner noted that while the Congress supports larger increases for NSF and continues to argue that the imbalance between the physical and the life sciences must be addressed, the reality was that this had to be considered in the light of a large national budget deficit, the war in Iraq, and the upcoming presidential and congressional elections. He noted that Congress has also expressed concerns about NSF's administration of the MREFC account. There is some talk that there will be no 2005 budget before the election, and some feel the FY 2005 budget may be a series of continuing resolutions.

Turner then turned to topics that would be discussed during this meeting. These included the second competition for the Approaches to Combat Terrorism (ACT) program, the pilot MPSAC Subcommittee for the Division of Chemistry, the Joint MPSAC/Education and Human Resources Advisory Subcommittee (JSAC), the just concluded MPS Cyberscience workshop, and the two Committee of Visitor Reports for the Division of Mathematical Sciences (DMS) and for the Division of Chemistry (CHE).

Turner noted that the National Academy of Sciences (NAS) Brinkman Report on NSF planning for major facilities had been received and that an NSF response to the Report is being prepared. The first report of the National Aeronautics and Space Administration (NASA) and NSF Astronomy & Astrophysics Advisory Committee (AAAC) had been submitted to Congress, to NSF, and to NASA. The Interagency Working Group Report on Physics of the Universe had just been issued.

The MPSAC commented on the response by the joint Department of Energy (DOE)/NSF High Energy Physics Advisory Panel (HEPAP) to a request by Turner and Dr. Robin Staffin, Associate Director of High Energy Physics Office at DOE, to define the goals of high energy physics. Dr. Janet Conrad commented that the community had not had input to the report and this was a problem. She wanted to know who had selected the big questions, and noted that it was not the community. Turner responded that about 15 to 20 people had participated in writing the report. Conrad said that while the report defined community goals, people in the community felt they had not been represented. As a result, part of the community was upset about the process by which the report had been commissioned. Turner said that the report had intended to show current investments, and was not intended to be a plan for future investment. It was not a prioritization process, but was a report on what was currently happening in this research area.

Turner also noted that there were ongoing studies such as the National Research Council (NRC) study on highenergy physics in the 21<sup>st</sup> century and the American Physical Society (APS) neutrino study. He noted the MPSled process for underground science. This field had been caught up in politics, but NSF had started the process moving again, and there were many potential MREFC projects in this area.

Turner commented that he was concerned about the status of the support for theory within MPS. A distinguished group of condensed matter theorists met with MPS, DMR and PHY, to address the challenges of being supported within "materials." Turner said that there have been no recommendations arising from that meeting but MPS had heard the concerns that this community was being ignored. Also, previous astronomy Decadal Studies had identified theory as an issue. He has had discussions on this subject with MPSAC members Dr. Thomas Appelquist and Dr. Roger Blandford. He suggested that perhaps there should be an MPSAC sponsored workshop that might be called "Theory in the 21st Century." How does one nurture theory, and he noted that the Kavli Institute for Theoretical Physics would be coming up for renewal soon. Pemberton suggested that MPSAC members think about this issue and about their own participation in such a workshop. This subject would be discussed by the MPSAC later in the day.

Blandford asked how earmarking was affecting NSF, since this was having a fairly significant affect at NASA. Essentially one entire mission a year in equivalent funding is being earmarked. He asked what the situation was at NSF. Turner responded that in FY 2004 approximately \$20,000,000 of the MPS budget of \$1,100,000,000 had been directed by Congress to be allocated to the National Radio Astronomy Observatory (NRAO) in AST and to the Rare Symmetry Violating Processes (RSVP) in PHY. Earmarking was a concern, but not yet a problem. Salah remarked that \$20,000,000 was not in the noise for any MPS division.

Dr. Gary Sanders was concerned about funding mid-scale instrumentation. He was concerned about how one was to provide funding for mid-scale instrumentation without putting pressure on individual investigator grants and how one was to prioritize mid-scale instrumentation for FY 2006.

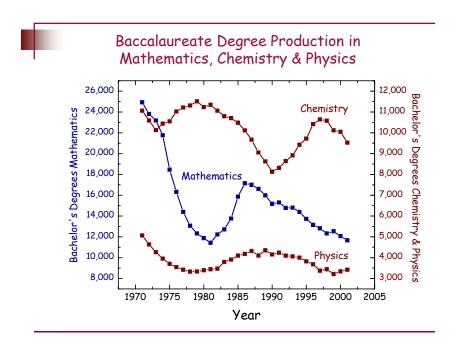
This concluded the budget discussion and a break followed at 10:15 AM.

# Joint EHR/MPS Advisory Subcommittee Report and Discussion on Education Activities and Work Force Issues

Pemberton began her presentation with a discussion of the recent history of the Education and Human Resources Advisory Committee (EHRAC) and MPSAC interactions. At the May 2003 meeting of the EHRAC, Pemberton presented, on behalf of the MPSAC, a proposal to the EHRAC for a joint study of undergraduate education in MPS. This proposal was endorsed by the EHRAC and led to the formation of an EHR/MPS Joint Subcommittee Advisory Committee (JSAC) whose membership was finalized during May – June 2003. During Summer 2003 a charge and initial work plan were developed by the Assistant Director of EHR and the Acting Assistant Director of MPS, and in Fall 2003, a liaison from the Directorate for Biological Sciences Advisory Committee (BIOAC) Subcommittee on Education was added. In addition, the EHRAC Chair was added to provide representation from community colleges. During Winter-Spring 2004 the initial stages of the study were implemented.

During Fall 2003, JSAC activities consisted of planning strategies and developing questions for focus groups. In Winter 2004, focus groups were created which met via teleconferencing, and in Spring 2004 the JSAC convened to assess its findings, develop preliminary recommendations, and prepare an interim report.

The question naturally arises as to why one wishes to focus on undergraduate education in the mathematical and physical sciences. The following diagram, which Pemberton presented, illustrates the creation of baccalaureates in the mathematics, chemistry and physics over the last 30 years:



Pemberton described the charge the JSAC had received from the Assistant Directors of EHR and MPS. The JSAC was charged with:

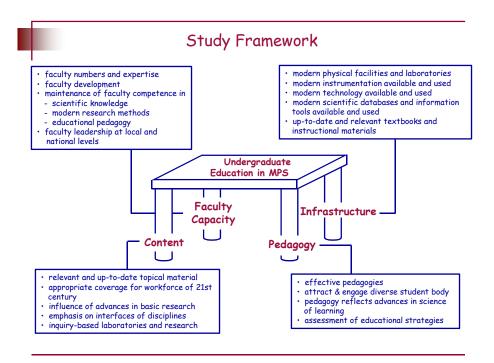
- 1. Examining the ways the MPS and EHR communities think about and describe the activities of research, professional practice, and education, and how those definitions affect the nature of their activities;
- 2. Exploring the commonalities and differences in approach of the two communities to integrating research, professional practice, education, and in defining successful integration; and
- 3. Recommending types of activities that EHR and MPS might undertake, either together or in parallel, that would
  - Strengthen preparation of the next generation of MPS professionals;
  - Broaden participation in the MPS disciplines; or
  - Create new pathways to MPS careers

either by building on existing programs, expanding them in directions that capitalize on commonalities of approach, or developing new programs that would promote innovative paradigms for the integration of research and education

In addressing the charge, the JSAC was to give consideration to:

- The current state of the undergraduate enterprises in chemistry, physics, and mathematics and how they are changing, with an emphasis on the integration of research, professional practice, and education;
- EHR and MPS activities with impact on undergraduate education and their efficacy in promoting change; and
- Past and current experiments in transcending the EHR-MPS boundary in carrying out these activities.

Pemberton illustrated the framework in which the JSAC carried out its initial study through the following diagram:



During December – February 2004, the JSAC was concerned with gathering data. It divided information gathering into three subareas:

- 1. Disciplinary communities in academia
  - Core disciplines of mathematics, chemistry & physics
  - Boundaries with other disciplines (e.g. biological sciences, materials science)
  - K-12 teacher preparation
- 2. Intersection of undergraduate education and professional practice (i.e. workforce perspective)
  - Industry, government laboratories
  - K-12 employers
- 3. Lessons from current and past undergraduate program and reform efforts

In February 2004, focus groups were created. Invitations were sent to approximately 350 scientists to participate in teleconference focus groups or to provide written responses to series of questions. Invitees were from core disciplines (mathematics/statistics, physics/astronomy, chemistry/biochemistry) and interface disciplines (biology, materials, environmental science). Invitees were from all sectors (academia [2-yr, 4-yr], industry, government labs, professional societies/non-profit organizations). As a result of these invitations, 49 individuals participated in the focus group teleconference, with 14 written responses, of which five were from teleconference participants. The majority of the participants were from the core disciplines in 4-year academic institutions. There was, it was felt, inadequate participation by workforce and two-year college faculty.

Pemberton then described the philosophy underlying the preliminary recommendations from the JSAC. It was that higher education is a dynamic, evolving institution, and that the forefront of undergraduate science education must continually evolve as high education evolves. Practice in undergraduate science education must be developed on the platform of an experimentally determined body of knowledge. Pemberton emphasized that one size does not fit all in undergraduate science education, that no "best" approach is waiting to be discovered, and multiple approaches will be contextually successful in different disciplines and institutions. NSF's challenge is to develop a rational, targeted process for experimental and evidence-based discovery of these approaches. Finally, she noted that ensuring evolution of the forefront of this body of knowledge would require a long-term, sustained commitment of financial resources.

#### The JSAC made 6 preliminary recommendations:

1) Issues and needs in undergraduate education in mathematics, chemistry, and physics can be quite distinct. EHR should experiment with discipline-specific programs that are developed with full integration of the expertise, insight into community culture, and understanding of the modern research frontier of the appropriate Division within MPS.

Pemberton commented that programs with uniform guidelines for all disciplines do not always address the most important needs in a given discipline; and programs for undergraduate education in MPS should be developed in a way that capitalizes on the relevant expertise in both Directorates.

2) Undergraduate reform efforts that engage the full range of faculty within a department and that seek to better infuse the current knowledge and modern professional practice of mathematics, chemistry, and physics into the undergraduate experience are likely to have the greatest positive impact on the education of majors in these disciplines. The development of a program to stimulate "department-level" reform in the undergraduate education of majors in these disciplines is recommended.

Pemberton commented that this recommendation was based on the holistic view that systemic change in undergraduate education for majors requires attention to the essential interdependence of the "four pillars" that were presented earlier. Furthermore, for better or worse, the academic department is still the functional unit of

educational change. Finally, the overarching goal is to engender broader faculty participation in ways that are institutionally defined

3) EHR and MPS should undertake activities to stimulate greater integration of two-year colleges with four-year colleges and universities in preparation of undergraduate majors in mathematics, chemistry, and physics; experimental approaches to addressing professional development opportunities for two-year college faculty are needed.

Pemberton noted that two-year colleges have a unique role as untapped resource of domestic students, especially underrepresented minorities. They are increasingly important in undergraduate education in mathematics, chemistry, and physics, especially for *affordable* lower division courses. It is important to note that communication between the two-year college and four-year institution sectors needs improvement to facilitate seamless student transfers. Also, faculty capacity at two-year colleges is suffering due to excessive teaching loads and professional development opportunities are needed for these faculty.

4) EHR and MPS should undertake activities to facilitate better integration of "researchers" and "educators" in mathematics, chemistry, and physics.

With respect to this recommendation, the JSAC felt that communities of "researchers" and "educators" in these disciplines, and their cultures, remain much too segregated and insular. There is a lack of cross-cultural knowledge, communication, and appreciation works to the detriment of undergraduate education in mathematics, chemistry and physics.

JSAC felt that EHR and MPS must deliberately seek mechanisms to foster greater cooperation between these two essential communities. EHR and MPS could:

- Require participants from both the "research" and "education" communities on "broader impact" activities on grants; and
- Proactively utilize representation from both communities on peer review of proposals from both Directorates
- 5) Greater integration of research and education in all EHR and MPS funding activities is needed to change the existing disciplinary cultures that value research over education and for more effectively engaging research faculty in the undergraduate education of majors in mathematics, chemistry, and physics.

JSAC felt there was a noticeable trend towards decreasing engagement of the most active researchers in undergraduate education. It was felt that the increased administrative burden associated with large center and group grants has contributed to this trend as faculty seek relief through release from teaching. JSAC thought that NSF should exhibit leadership in mandating participation in undergraduate education as a high-priority responsibility of its funded academic research faculty.

6) EHR and MPS should consider exploring changes in staff organization to better facilitate educational activities between the two Directorates. As an example, EHR and MPS might explore the establishment of a staff position/office charged with integrative educational activities between the two Directorates with dual reporting lines to the EHR and MPS Assistant Directors.

Pemberton commented that this recommendation was modeled on the successful MPS Office of Multidisciplinary Activities (OMA). It was important that such activities be *funded by and answer to* both the EHR and MPS Directorates. Furthermore, integration of appropriate research and education activities across the EHR/MPS boundary could significantly enhance impact of the NSF investment in undergraduate education in the MPS disciplines.

After presenting these interim JSAC recommendations, Pemberton provided a rough timeline of future JSAC activities. Following the interim report acceptance and feedback from the EHRAC and MPSAC, JSAC would carry out data gathering through Phase II focus groups during Summer 2004. It would make an assessment of findings, formulation of final recommendations in September 2004. Final report preparation would take place

during October 2004, and final report approval would be requested from the EHRAC & MPSAC at the November 2004 meetings of these two advisory committees. Final report submission to the EHR and MPS Assistant Directors would take place in November 2004, with future JSAC activities decided by EHRAC and MPSAC.

In the discussion that followed Pemberton's presentation, Dr. Jon Kettenring noted that mathematics appeared to stand out in terms of the loss of majors and asked if Pemberton understood the root causes of this and if the subcommittee had any recommendations that stood a chance of turning this around. Pemberton responded that the cause of this problem in mathematics was that students find undergraduate mathematics irrelevant, with no connection to the real world. There was a strongly held opinion that research mathematics should be part of undergraduate education. Huchra commented that there seemed to be a connection between enrollment in mathematics and the increase in computer science enrollment. Pemberton replied that the mid-1980's rise and fall in mathematics enrollment was coupled with the computer sciences rise but it was not that simple.

Huchra expressed disappointment at seeing so little contribution to this effort from his astronomy colleagues, and Pemberton responded by saying that the subcommittee would continue to seek their input. Dr. Mostafa El-Sayed asked about enrollment in biology. The response was that enrollment in biology had doubled in the 1990s and 64,000 bachelor's degrees in biology are awarded every year. Dr. Janet Conrad asked about new students and the number interested in wanting to seek careers in science, engineering and mathematics. Pemberton stated that the percentage of students expressing interest in these fields when they enter as undergraduates has remained fairly steady, but the percentage that actually receives degrees has gone down. Blandford was critical of what is currently being taught in mathematics departments in the sense that there is a reduction in emphasis on what is rigorous proof, and felt it was important that this not be lost.

Turner noted that integration of research and education is a major theme at NSF, and was distressed with recommendation 5. What is the evidence for this disconnect? Pemberton responded that the decadal mathematics survey showed that the numbers of faculty in undergraduate education are decreasing. Other areas are not so clear; some of the evidence is anecdotal. Turner still felt the subcommittee recommendation was troubling, and wondered why directors of centers were singled out. He did not believe that the centers removing people from teaching was a problem. Pemberton responded that the subcommittee had no intention of singling out centers. It was not administrative burdens that were the sole cause of this problem – the buyout of teaching by using research dollars is rising. NSF should emphasize the research/education connection, and should not neglect its importance. Turner still felt that the conclusion was not true. Dr. Frances Hellman felt that if this were true, the statements should be backed by evidence, and not be anecdotal in nature.

Dr. Shenda Baker noted that not all researchers are good educators and one should be careful about blanket statements. If there were fewer researchers in teaching, were they involving undergraduates in their research? Pemberton responded that the involvement in undergraduate education is not always in the classroom. Undergraduate research is a good example. Dr. Gary Sanders commented that most centers have outreach and undergraduate research, and their net effect is likely to be positive. Hellman supported Baker's comment concerning Research Experiences at Undergraduate Institutions (REU). She noted that NSF has made a major effort in this area, that this should be continued, and there was a need for more statistics as to undergraduate participation in research. While undergraduates are often listed in detail in the reports for an award, they are not listed in proposals. Pemberton responded that in a recent survey of graduating college seniors, of those in the physical sciences, only ~25-27% reported having a research experience with a faculty member. Huchra noted that numbers were clearly location dependent - smaller colleges often have no research, while major institutions may place every undergraduate in a research activity. Dr. David Morrison commented that there were also disciplinary differences, with different teaching loads and different buyout practices. One could not generalize. Hellman thought that one might want to encourage students to have research experience in their first year, but at many institutions there was considerable resistance in involving freshmen in research. Could the JSAC study recommend such an option? Pemberton responded that it was included in the text in the context of the URC program as a model.

Turner felt there was a real focus by universities to encourage the participation of undergraduates in research that was not well reflected by the wording in the text as written in this report. Morrison noted that it was harder

to get undergraduates to do research in mathematics. Turner commented that NSF did not want individuals receiving NSF support to be exempted from teaching, and much of the effort MPS is putting in this area is not reflected in the report. Pemberton responded by saying that the subcommittee would revisit this area and would check the wording of Recommendation 5.

Dr. Lucy Fortson thought that the group of informal science centers should contribute to this study, as well as undergraduate centers, and stated that she would be happy to become involved in this activity. Pemberton thought this was an excellent idea, and that she would welcome having a list of individuals she could contact. Salah was concerned by the poor response to the survey, and wondered why this was happening. Pemberton thought that it might be due to not enough interest or concern in undergraduate education. Appelquist stated he was glad to see the emphasis on two-year colleges in the report. Aizenman commented that there had been recent articles in the press concerning attendance at two-year colleges, and that there were financial reasons for students choosing two-year colleges as their entry into undergraduate education. Pemberton commented that 30-35% of degree recipients take at least one course at a 2-year college, and that number is increasing.

Fortson asked about how input was solicited for the report. Pemberton responded that individuals were sent emails with several possibilities of specific times for participation in the focus groups, but it was logistically impossible to be completely flexible. Kettenring asked whether any statisticians had been involved. He noted that the American Statistical Association should be delighted to help. Pemberton responded that the list of responders was in the report, but asked for the names of additional people. Dr. Jean Futrell asked if JSAC was planning to hold further focus group meetings. Pemberton responded in the affirmative, saying these would be held this summer to fill in the blanks.

Pulleyblank thought that the report had to have a few specific action recommendations and suggested that the report name "the top three things we could do." Turner commented that this would be extremely helpful.

Bob Hilborn, a member of the subcommittee, thanked everyone for their comments and wanted to thank Pemberton for her "heroic efforts" on this activity. Applause from the entire audience greeted this remark.

#### Report of the MPS Cyberscience Workshop of 04/21/04

Baker presented an overview of the MPS Cyberscience workshop that was held April 21, 2004. The purpose of the workshop was to identify needs for cyberscience, defined as the science that cannot be done without the advanced capability of cyberinfrastructure. The morning session consisted of six invited speakers drawn from the MPS disciplines, each presenting "science drivers" as illustrated by their own research. The afternoon consisted of several breakout sessions organized around common themes. The evening session stressed commonalities across the MPS disciplines.

There was representation from all of the division in MPS, and the workshop began in the morning with six invited talks. The speakers were Dan Reed of North Carolina State University, Larry Smarr of the University of California at San Diego, Alex Szalay of Johns Hopkins University, Brent Fultz of the California Institute of Technology, Vijay Pande of Stanford University, and David Keyes of Columbia University.

The breakout sessions in the afternoon consisted of needs associated with 1) algorithms and software; 2) software infrastructure; 3) hardware and facilities; 4) network Infrastructure; and 5) data management and infrastructure.

Baker commented on the talks given by the invited speakers. Reed, in quoting others, had noted "the purpose of computing is insight, not numbers (Hamming)" and commented on computing for science versus computing as science. Szalay described how discoveries are made at the edges and boundaries of science, that the utility of computer networks grow as the number of possible connections, that the internet and grid tools are converging, and that optimization of searching is needed (software and algorithms). Keyes had discussed whether simulation can produce more than "insight" and had quoted J.S. Langer as "The computer literally is providing a new window through which we can observe the natural world in exquisite detail." He also noted that Ray Orbach, Director of Science at the Department of Energy, has stated that the ITER design of plasma reactor would be

capable of achieving fusion based on a simulation. Brent Fultz, in discussing neutron scattering, had discussed the need to build software systems and had described data reduction, direct comparison to simulations of the detector in real time, direct visualization and data archiving. Vijay Pande had described work on protein folding and the coupling of theory, simulations, and experiment. He stated that the computer models must provide insight and not just reproduce experiments. Since timescales of molecular motions are fast (of the order of femtoseconds), following such motions takes a long time. Computations are done via distributed computing on public machines much like "SETI at Home."

Recommendations that resulted from the workshop were the following:

- 1. There is a need for development of tools for cyberscience that would support science research and sit on the cyberinfrastructure being funded by NSF. An SBIR-like process should be developed for support of such development, with successful Phase 1 projects leading to further support as Phase 2 projects;
- 2. There should be a reallocation of a portion of the NSF budget to support cyberscience awards, with supplements to proposals with cyberscience tool components;
- 3. MPS should add a cyberscience component to its web page; and
- 4. There is a need for coordination of cyberscience and cyberinfrastructure and this must be addressed "up front."

Finally, the workshop concluded that long-term support for people in infrastructure should not be an MPS role.

Blandford commented that because of hardware and software implications, it is important to emphasize that one size does not fit all. The rate-limiting step is not access to central processing unit time, but the people themselves, *e.g.*, writing poor code. NSF could invest in the people in that area between computer science and science, and tap that capacity.

Sanders commented that at the workshop there were articulate, talented people pushing a new view. It is "algorithms" that need the investment, not "computer cycles." Investing in software means investing in people, and that is expensive. We have moved away from the model of the supercomputer center, and now assistant professors are running their own Beowulf clusters. The NSF Small Business Innovative Research (SBIR) Phase I/Phase II model should be explored.

Fortson asked how one could balance the needs for standards versus "letting a thousand flowers bloom." Pulleyblank responded that cyberscience rests on cyberinfrastructure but has no other restrictions. One should try various approaches and see what succeeds. Dr. Mitch Waldrop from NSF's Office of Legislative and Public Affairs commented that rather than imposing a standard from the top, an alternative is to debate different ideas, test codes, and converge on a standard. This is a community-driven, bottom-up process. Baker agreed, but wondered as to how one would then facilitate communication across different communities.

Pemberton noted that a factor that was missing was how cyberinfrastructure overlaps with education. She gave as an example access to modern instrumentation and virtual experiments. Kettenring commented that tools like visualization were discussed in breakout sessions at the workshop and one should look at NSF's Directorate for Computer and Information Science and Engineering's (CISE) efforts here. Pemberton responded that there was also simulation in addition to visualization, and that the science that is done in these areas will map onto educational needs.

Sanders noted that the workshop had ended with the direction that a component of cyberinfrastructure must reside within MPS and it must not be treated as computer science research. In fact, he felt that there had been impressive, specific examples in the breakout sessions, more so than in the morning invited talks. Pemberton added that it had been a stimulating workshop, and it was extraordinary that recommendations came out of just one day.

Turner noted that Dr. Peter Freeman, the Assistant Director for CISE was present at the meeting and asked if he (Dr. Freeman) wished to make any comments. Freeman said that the workshop had been productive and that things are headed in the right direction. He commented that one should think of the CISE budget as that of a

computer center plus a computer science department, and these are two very different organizations. One doesn't know what many MPS scientists need, so this generates good computer science research.

Turner commented that there was discussion within NSF to create, within CISE, an Office of Shared Cyberinfrastructure that was to be responsive to scientists of all disciplines. He noted that within MPS, investments in Information Technology Research (ITR) amount to approximately \$35,000,000. If NSF were to begin a cyberinfrastructure initiative, then MPS will have the \$35,000,000 plus an additional amount to invest in various areas. For example, it has been suggested that software is where MPS should invest. How would one do that? Morrison thought that if principal investigators receive a supplement for cyberscience development activities, one might consider requiring that such development be usable by the broader community. Pemberton suggested that this issue be discussed within the divisional breakout sessions that afternoon.

#### Update on Approaches to Combat Terrorism (ACT)

Dr. Adriaan de Graaf summarized the history, recommendations and implementation of the Approaches to Combat Terrorism (ACT) Program, which is a joint program between MPS and the US Intelligence Community (IC). The Intelligence Community is defined as parts of 14 agencies (see <a href="http://www.intelligence.gov/1-members.shtml">http://www.intelligence.gov/1-members.shtml</a>)

In July 1998 the U.S. Commission on National Security/21st Century (USCNS/21) was chartered by Secretary of Defense William Cohen and on February 15, 2001 the Commission issued the third and last of its reports "Road Map for National Security: Imperative for Change" (the Hart-Rudman Report) that contains an extensive analysis of the current capability of the United States to respond to threats to homeland security as well as the strength of the national scientific enterprise.

The report made significant recommendations for improvements in these areas, including an enhanced role for the National Science Foundation in the stewardship of the national scientific research and education programs. In November 2001 the MPSAC reviewed the issues in the Hart-Rudman report and focused on the areas of *Improving Homeland Security* and *Recapitalizing America's Strength in Science and Education*. The MPSAC formed a subcommittee chaired by Pulleyblank to address ways in which MPS can respond to the recommendations of the Hart-Rudman report. At the May 2002 meeting of the MPSAC, the subcommittee presented a white paper that made specific recommendations to MPS. These recommendations were:

- 1. The National Science Foundation, and in particular, the MPS Directorate, should expand its role as a steward of America's science research capability. NSF/MPS should continue to focus on its strength in basic research, while responding to issues of national priority, such as homeland security and science education.
- 2. The MPS Directorate should play a leadership role in convening a strategic meeting with other agencies to discuss domains of interest and to establish means of coordination of activities.
- 3. The MPS Directorate should create and maintain an inventory of the research activities and capabilities in the fields that it covers. The inventory would start with current and recent grant awardees, but subsequently should be expanded. Having such an inventory will enable an assessment of existing activities and their support.
- 4. The MPS Directorate should take actions that will support the formation and maintenance of an active, national community involved in carrying out research in areas relevant to homeland security: Actions could include workshops, communications at national meetings and solicitations for exploratory proposals.
- 5. The MPS Directorate should conduct a set of open workshops to define actions that will support the recapitalization of America's strength in science and education. A cross-directorate Steering Committee should be formed to plan these workshops. The result of these workshops should be a detailed implementation plan.

De Graaf noted that MPS had implemented all of the subcommittee recommendations, with the exception of recommendation 3.

In the summer of 2002, MPS began discussions with Intelligence Community (IC) on ways in which MPS could work with the IC community in common areas of interest. Five areas of research were identified as being of interest both to MPS and to the IC. It was decided that a workshop, jointly supported by MPS and the IC, would be held at which members of the academic community would meet and discuss these topics. On November 19-21, 2002 a workshop entitled "Approaches to Combat Terrorism (ACT): Opportunities for Basic Research" was held in Virginia. Dr. Ernie Moniz of the Massachusetts Institute of Technology (MIT) and Dr. John Baldeschwieler of the California Institute of Technology were co-chairs of the workshop. During the early months of 2003, as a result of the workshop, MPS and the IC issued a solicitation for supplements and for Small Grants for Exploratory Research (SGERs) to conduct research in the areas identified by the ACT workshop. MPS provided \$2,500,000 for this effort and the IC provided \$1,000,000. The IC funds were transferred to NSF. In response to this solicitation 157 requests were received. After a joint review conducted by MPS and IC staff 39 awards were made during the summer of 2003. By Fall 2003, preparations had begun for a second round of proposals (ACT II). In March 2004, an ACT II solicitation for SGERs was issued. (http://www.nsf.gov/pubs/2004/nsf04561/nsf04561.htm). Support for this solicitation is \$2,500,000 from NSF and \$1,000,000 from the IC. The submission deadline is June 11, 2004. NSF anticipates making 15-20 awards up to a total of \$200,000 each.

De Graaf stated that the future of the ACT program is not determined at this time.

In the discussion that followed this presentation, El-Sayed asked if principal investigators from last year's competition are allowed to submit this year. De Graaf replied that there is no restriction on eligibility in this way. El-Sayed asked if there was any restriction on publication. There is none.

Several MPSAC members asked why the IC contribution was so much smaller than that from NSF. Turner commented that perhaps the contributions from NSF and the IC should have been equal. The ACT program has the right features – it is transparent and that while MPS wants to do something that works for the IC it is not obvious that this works for them. For example, peer review takes time, and fast decisions (like at DARPA) might be important to the IC. Turner added that Freeman was coordinating NSF's effort on national security. He thought that the MPSAC might want to make a statement that the MPSAC supports, in principle, basic research for national security, and that there is a need for an evaluation of ACT. He wondered what other mechanisms could be used to help cross-fertilize the MPS and IC communities? El-Sayed suggested workshops. Baker saw this program, or some version of it, as a development opportunity for the MPS community. The Strategic Defense Initiative (SDI) example is not apt because at the time, scientists did not believe SDI would work. However, scientists are optimistic about making gains in science and technology to improve national security.

The meeting was adjourned for lunch.

Thursday, April 22, 2004 Afternoon Session

#### **Divisional Meetings**

During the afternoon subgroups of the MPSAC met with the individual MPS divisions in breakout sessions. The full MPSAC reconvened at 4:00 P.M. to begin a discussion of long-range planning.

#### Discussion of Brinkman Report on Facilities

The MPS Advisory Committee reconvened at 4:00 PM.

Pemberton announced that the next day's meeting would convene at 8 AM, that the Chemistry breakout report would be heard from 8:00 - 8:30 AM, to be followed by the Physics breakout report from 8:30 - 8:45 AM, and

this would be followed by the Division of Chemistry Committee of Visitors report at 8:45 AM.

Turner described the recently released report by the National Academy of Sciences chaired by William Brinkman (retired) of Princeton University's Department of Physics entitled "Setting Priorities for Large Research Facility Project Supported by the National Science Foundation <a href="http://books.nap.edu/html/lrf">http://books.nap.edu/html/lrf</a> projects/0309090849.pdf." Congress had requested the report. Key issues raised in the report included the transparency of the NSF process and involvement of the community (especially advisory committees) in the selection of projects. Of greatest concern was whether NSF had a roadmap for this process, given the existence of the 20-year long-range plan of the Office of Science within the Department of Energy. Turner noted that DOE provides 60% of the federal support for basic research in the physical sciences and that they support a large number of facilities.

Turner felt that a shortcoming of the report was that it did not discuss differences between NSF and DOE. NSF would not do a 20-year roadmap, as that would eliminate flexibility. He said that NSF could have a "three-basket model," *i.e.* ready-to-begin, almost ready, and on the horizon (blue-sky). He noted that NSF had a Deputy Director for Large Facilities whose role was to maintain oversight of the NSF process for facilities but that the NSF Directorates and Divisions carried out direct oversight of a facility. In many cases there were program officers whose full-time activity was associated with oversight of a facility. The role of the National Science Board (NSB) was to validate the process and provide a check on these activities. Furthermore, the design and development funds for a proposed facility, estimated to be about 10% of the total construction costs, was the responsibility of the Directorates/Divisions.

Turner commented that the report did not address life-cycle costs. Maintenance, upgrades and other costs could, over the lifetime of the facility, come to several times the original construction cost. This funding has to come from divisions/directorates – there is no line for this in the budget. However, this would not be part of the NSF response to the report since such topics had not been covered in the report.

The NSF response to this report was due in early Fall 2004. There would be both an NSF and an NSB response. There were two items which the response would have to pay particular attention to: transparency—NSF had to articulate the process, which Congress does not understand, and the question of a roadmap—which NSF did not have at the present time. Such a roadmap should say how facilities are prioritized and selected, which are almost ready for selection, and which are still somewhat "blue sky."

Turner then described the NSF Major Research Equipment and Facilities Construction (MREFC) approval process. Ideas come from the community in the form of proposals, undergo Divisional/Directorate Review, are then reviewed by NSF, undergo addition review by the NSF Director's Review Board, and, if this review is satisfactory, are approved by the Director for consideration by the NSB. After review, the NSB may approve the project for inclusion in "the queue." They are subsequently approved by the Director and the NSB for inclusion in the President's budget request to Congress. If Congress appropriates funds for the project, NSF, through the Director and the NSB, approve an award when appropriated funds are available.

Turner noted that IceCube is a MREFC project that is ready to go to the NSB for budget approval and that the Rare Symmetry Violating Processes (RSVP) project is in the President's FY 2005 budget request. The Advanced LIGO project has been approved by the Director and has been forwarded to the NSB.

In the discussion that followed this presentation Sanders noted that the Brinkman Report had presented the DOE roadmap process as a paradigm that NSF could adopt. Turner responded that prioritizing different kinds of facilities is comparing apples and oranges. He noted that once a project was within the NSF queue, it is not removed. However, Congress has asked NSF to reexamine the current order within the queue.

#### Discussion of Directorate Long-Range Planning

This session of the MPSAC meeting began with a presentation by Turner on Directorate activities involving long-range planning since the November 2003 meeting of the MPSAC. There had been a half-day meeting in January with MPS Program Directors, a half-day meeting with MPS Division Directors, and a two-day retreat by

MPS senior staff on this topic. He noted that the process was still not complete.

Turner began by noting that at the MPS retreat staff had developed the following MPS mission statement:

"To make discoveries about the Universe and the laws that govern it; to create new knowledge, materials, and instruments which promote progress across science and engineering; to prepare the next generation of scientists through research, and to share the excitement of exploring the unknown with the nation."

Within this mission, the Directorate science themes that were developed were:

- Charting the evolution of the Universe from the Big Bang to habitable planets and beyond
- Understanding the fundamental nature of space, time, matter, and energy
- Creating the molecules and materials that will transform the 21st century
- Developing tools for discovery and innovation throughout science and engineering
- Understanding how microscopic processes enable and shape the complex behavior of the living world
- Discovering mathematical structures and promoting new connections between mathematics and the sciences
- Conducting basic research that provides the foundation for our national health, prosperity, and security

These scientific themes had been developed because of their scientific opportunities. Pemberton asked if there had not been something about the workforce that had been in the list at the November meeting, and Turner responded that these were the science themes. Narayanamurti thought that "workforce" might belong in a theme about preparing the next generation of scientists. Turner then described each of the seven science themes in terms of where we currently are, where we are going, and the major science questions in each theme.

Turner then described the discussion that had taken place at the MPS retreat concerned with defining the "core." The core is considered the heart of what MPS supports; yet it is difficult to define. In terms of definitions, all of the MPS divisions agreed that the core consisted of individual investigators and groups submitting unsolicited proposals. However, whether centers and facilities should be included differed among the divisions. A similar situation existed with respect to NSF priority areas. Other definitions of the core included what program officers "control," unfettered, discovery-driven research, and what "the community wants us to protect."

The retreat had discussed current MPS facilities and related mid-scale projects. In considering what facilities and mid-scale projects would be supported, the primary criteria that should be considered were those of:

- 1) Scientific excellence (the science should be transformational and at the cutting edge):
- 2) The facility or project should be enabling, in that it was needed by a large community and performed an essential scientific function;
- 3) The facility or project was ready in terms of technology, management, and leadership; and
- 4) It was appropriate for NSF to have a role in support of this facility or project in terms of world leadership, preparing the next generation, *etc*.

Additional factors that had to be considered in considering what facilities and mid-scale projects to support included supporting research and development activities related to getting the project ready, the impact of operations of a new project or facility on other activities, the need to retire or transition current facilities as the new facility came on line, the need for an accurate assessment of lifecycle costs, and the need to prioritize within divisions, across MPS, across NSF, and in the interagency and international contexts using consistent criteria and taking other needs into account.

Turner then turned to a description of a list of *possible* facilities that were being considered in the context of "where do you want to be in 2020 with realistic funding growth." These included:

- Advanced LIGO estimated cost of \$140,000,000 estimated earliest possible start (EEPS) is 2006;
- Underground Laboratory estimated cost of \$300,000,000 EEPS is 2008;

- Energy Recovery Linac (ERL) estimated research and development (R&D) costs of \$40,000,000 EEPS is 2006;
- X-ray-FEL estimated R&D costs of \$15,000,000 EEPS is 2006;
- X-ray FEL estimated construction cost of \$300,000,000 EEPS is 2009;
- Advanced Tech. Solar Telescope (ATST) estimated cost of \$160,000,000 EEPS is 2005;
- Large Synoptic Survey Telescope (LSST) estimated R&D costs of \$14,000,000 EEPS is 2005;
- Large Synoptic Survey Telescope (LSST) estimated construction cost of \$140,000,000 EEPS is 2008:
- Giant Segmented Mirror Telescope (GSMT) estimated R&D costs of \$40,000,000 EEPS is 2006;
- Giant Segmented Mirror Telescope (GSMT) estimated construction cost is \$900,000,000 EEPS is 2012;
- Enhanced Very Large Array II (EVLA II) estimated construction cost is \$120,000,000 EEPS is 2012:
- Square Kilometer Array (SKA) estimated R&D costs of \$25,000,000 EEPS is 2006;
- Square Kilometer Array (SKA) estimated construction cost is \$1,000,000,000 EEPS is 2015;

Baker asked if there was money for all these facilities. Turner replied that at the moment the only commitment is \$10,000,000 to the Advanced Technology Solar Telescope (ATST).

Pemberton asked Turner what he expected of the MPSAC with respect to these possible projects. Turner replied that he wanted to know what the MPSAC thought of these projects, and Sunley added that MPS would have to make R&D commitments in the near future. Baker noted that the projects seemed to consist of physics and astronomy projects and wondered if the MPSAC was the right group of individuals to provide input to Turner on these proposed projects

Turner also discussed decision criteria that had to be used in making choices on proposed projects. These included the impact on current facility operations, assessment of life-cycle costs, and the reuse or transfer of current facilities.

Turner then discussed workforce issues. He noted that diversity in the workforce was becoming increasingly important. There was also the current policy concerning the issuing of visas to foreign scientists and students wishing to enter the United States that appeared to be discouraging foreigners from studying here. Workforce goals for MPS included doubling the number of undergraduates in research experiences in MPS, attracting talented middle/high school students and have 'MPS discovery' inspiring them to pursue MPS subjects, extending Research Experiences for Teachers (RET) activities to engage K-12 students, developing and implementing an integrated research model for MPS undergraduate education, and having an impact on 2-year institutions via contact enrichment and attracting underrepresented groups.

Dr. Carl Lineberger asked about the costs of carrying out all of these proposed projects, and estimated it would cost about \$10,000 per student. Turner suggested that supplements could be offered to researchers who employ undergraduates, particularly undergraduates from underrepresented groups.

Turner then discussed the preparation of the MPS FY 2006 budget request. He noted that items that had to be considered included workforce, diversity, nurturing the core, advanced LIGO, and ATST. There was also the question of cyberinfrastructure. The NSF FY 2006 budget request would be sent to OMB the first week of September, with a response expected from OMB by Thanksgiving. Sunley noted that this was the last opportunity for the MPSAC for input into the budget.

In the discussion that followed, Pemberton commented that information on these matters should be provided to the MPSAC in a more appropriate format, along with estimates of costs, and that it was difficult to decide such issues in the short period of time that remained. Conrad said that the MPSAC needed more information to assess what items it should recommend to MPS. Baker stated that flat budgets were probably with us for some time, and so there is need of prioritization. Huchra felt that more information was needed by the MPSAC.

Baker thought that the MPSAC could recommend activities in cyberscience and a few other topics. It was difficult for the MPSAC to decide which projects should get design and development funds, but

workforce/diversity issues and nurturing the core would be easier for the MPSAC to discuss. Pemberton felt that the MPSAC had numerous details in front of it, and that support of the core was more important than cyberscience.

Blandford commented that to many the manner in which NSF spent large sums of money was somewhat mystifying, and what Turner was doing was an attempt at demystifying the process. He (Blandford) was very glad that this process was being opened to the community. It was clear that R&D support would go to more projects than would actually end up being constructed. He suggested that all of the projects that had been discussed received R&D support, other than those that might be supported by the Department of Energy.

Huchra thought that the core should increase at least as fast as inflation, and in this context he defined the core as unrestricted research. As far as cyberscience was concerned, the major need for resources was in the area of archiving and data storage.

Pemberton felt that a process by which such input to MPS was provided needed discussion and revision. Conrad thought that the MPSAC might break up into subgroups to examine the projects. Hellman felt that one should have worked from the findings of the breakout groups. Morrison noted that what was being requested was endorsement from the MPSAC, wondered how their advice could be useful, and commented that the MPSAC had not been oriented as to what they should be doing.

Fortson commented that at the November meeting the MPSAC had identified items on which advice could be given. She thought that by breaking into three or four groups a strategy for priority setting could be developed. Such a process could be important for everyone. Conrad agreed. Sunley noted that the various areas of the budget do not exist in isolation. Projects that involve cyberscience or cyberinfrastructure will have an impact on a broad range of science programs. For example, Physics of the Universe programs could involve many things beyond individual grants.

Turner commented that one could look at the priorities and see if everyone was in agreement. Facilities are a major item in MPS budgets. However, everyone agrees that the core is important, and, this being the case, perhaps identifying its elements would be useful.

Baker stated that there had been four specific recommendations made with respect to cyberscience. Sunley felt that while the group could agree on priorities, it might not do so on specific recommendations. Turner thought that subgroups of the MPSAC should be formed, with each group dealing with a specific topic. Pemberton commented that since the MPSAC would be hearing from the Division of Chemistry breakout group in the morning, it would a useful plan for looking at the future.

#### Adjournment

The meeting was adjourned at 5:45 P.M.

#### Friday, April 23, 2004

Morning Session

Pemberton convened the meeting of the MPSAC at 8:00 am.

#### Long Range Planning: Reports from Divisional Meetings

(Membership within each breakout group can be found in Appendix II and the reports from each of the breakout sessions are found in Appendix III.)

Division of Physics (PHY)

Appelquist reported on the Division of Physics (PHY) breakout session. Dr. Joseph Dehmer, Director of the Division of Physics had provided an update on PHY activities. Approximately 50% of the funds are provided to

core activities, about 33% go to facilities, and the remainder to centers and other activities. The breakout group discussed the balance of funding within the division, and it appeared that the theory programs are being stressed. There are 13 Physics Frontier Centers (PFCs) and the next round of proposals for PFCs are due in August 2005. PHY anticipates funding approximately two medium-sized PFCs per year.

With respect to facilities in PHY, it is anticipated that the Cornell accelerator will be shut down in the FY 2007/FY 2008 timescale. In terms of operational support for facilities, if one assumes a growth of the PHY budget of 3% per year, then PHY should be able to fund everything except for operations for the Large Hadronic Collider (LHC) and an underground laboratory.

The Rare Symmetry Violating Processes (RSVP) project will receive \$6,000,000 in FY 2004, and \$30,000,000 in FY 2005. The total cost of the project will be \$150,000,000. PHY is recruiting program directors for RSVP and for the nuclear theory program. The situation with respect to staffing in PHY is better than it was a couple of years ago.

The MPSAC breakout group was unanimous in its opinion that an underground laboratory was important but that it cannot be funded by PHY alone. With respect to cyberscience and cyberinfrastructure, PHY expects to spend about \$7,900,000 in this area. Appelquist noted that with respect to workforce/outreach activities in PHY, there are large education and outreach efforts via Quarknet, the Large Hadronic Collider, and RSVP. PHY has about 50 Research Experiences for Undergraduates (REU) and (Research Experiences for Teachers (RET) sites. The Physics Frontier Center at Hampton University has a large number of minority participants.

Turner commented that no decision has been made to fund an underground laboratory. Within NSF there is a working group of program officers from the different directorates having an interest in the creation of such a laboratory. Operational costs are a worry.

Division of Chemistry (CHE)

#### a) MPSAC Chemistry Subcommittee Meeting of March 16, 2004

Futrell reported on the experiment that had been conducted by the MPSAC in creating a Chemistry subcommittee that Futrell chaired. The subcommittee met with the Division of Chemistry for an entire day on March 16, 2004 This meeting provided a more thorough insight into activities of CHE than is possible at the shorter breakout sessions at regular MPSAC meetings and everyone who had participated in the meeting considered it to be a great success.

Futrell proceeded to describe the meeting, which began on March 15 with dinner followed by a talk by Walt Stevens of the Department of Energy (DOE). Stevens described the differences between DOE and NSF and the distortions of budgets that had been caused by the huge increases at the National Institutes of Health (NIH) compared to the relatively flat funding for DOE and NSF. On March 16 the Chemistry Division Committee of Visitors report was discussed. Turner joined the subcommittee at that point to discuss CHE priorities. However, the subcommittee did not feel qualified to set priorities for the chemistry community as a whole. The chemistry community does not have a single body that sets priorities like other fields do. The subcommittee felt that there is an important role for CHE in cyberscience and cyberinfrastructure.

Futrell commented that the subcommittee meeting established good rapport and understanding of problems faced by CHE Program Officers. He encouraged other disciplines within MPS to consider similar meetings Pemberton seconded these comments, and noted how useful the extended interaction had been.

#### b) MPSAC Chemistry Breakout Session

Ellis described the discussions that had taken place during the breakout session. Cyberinfrastructure and cyberscience were not quite on the radar screen of chemistry community. The recent MPS workshop on cyberscience had identified opportunities such as data access; data visualization; and other topics as well as the possibility of doing distributed processing of large problems in a manner similar to that of "SETI at home."

With respect to the core areas of support, 70% of the CHE budget is allocated to individual investigator funding. Centers could be considered part of core, but this would not be the opinion of the entire chemistry community. The discussion at the breakout session led to the thought that perhaps partnering with other NSF divisions/directorates, and other agencies including DOE and NIH could enhance core support. Chemical imaging of single molecules is one highlighted possibility; and a workshop might lead to mid-scale funding of cyberinfrastructure issues.

With respect to the workforce, there is interest in involving high school students in chemistry activities. CHE has an extensive REU program. The Discover Core Fellowships: funds mid-career changes that support public service activities. At the American Chemical Society (ACS) Fall meeting there will be a poster session for new faculty candidates, and this may make faculty recruiting more efficient. With respect to outreach and engaging the community, Dr. Luis Echegoyen will be submitting a proposal to the ACS to hold a poster session at an ACS meeting that will highlight exhibits on broader impacts.

Turner commented that the MPSAC Chemistry Subcommittee experiment had been valuable. He thanked the subcommittee for helping him understand that increased NIH funding for chemistry may actually be hurting the field by causing it to focus too narrowly on biochemical research. Other divisions may want to consider their own broader impact poster sessions.

An MPSAC member commented that many universities are setting salary based on NIH requirements, which may not be consistent with requirements and goals of the physical science.

#### Committee of Visitors (COV) Report on the Division of Chemistry

Dr. Robert Silbey of the Massachusetts Institute of Technology, Chair of the COV, presented the COV report for the Division of Chemistry.

The COV found that CHE was operating well both in terms of the quality of science it was supporting and the manner in which it was administering awards. There has been a large increase in the number of proposals handled by CHE, and this has significantly increased the workload of staff. The COV found the program directors very knowledgeable about the areas for which they have responsibility.

As to the awards themselves, the COV was strongly supportive of the single investigator awards, infrastructure and instrumentation, and REU awards that had been made by CHE. The quality of research at undergraduate institutions and REU sites supported is high. Silbey commented that a large number of undergraduate students want to participate in the type of research being conducted, and there is an increase in interest among the undergraduate students in participating in research at the interface between chemistry and biology/biochemistry. In this regard there is a large disparity between the size of NIH and NSF awards. NIH is increasingly supporting chemists, and biologists are moving into biochemistry-related research.

In discussing the statistics of awards supported by CHE, Sibley noted that CHE awards support 1600 graduate students and 600 postdocs. Of these, 16% of the principal investigators (PIs) and Co-PIs are women. This is particularly commendable since the percentage of women chemists in the U.S. is approximately 12%. Five percent of the CHE awardees are from underrepresented and minority groups.

With respect to the future, Silbey commented that cybertechnology programs (including the distribution of software) would connect the general public with the excitement of forefront research in chemistry. He gave biochemical reaction networks as an example of an emerging area that would provide a launching pad for the chemistry community. Chemical imaging was mentioned as the strength in the community. Also, the intersection of biology and chemistry (cusp) is where chemists can play an important role. But there is a concern that chemists don't get "respect" and therefore, efforts to do a good job of "selling" – *i.e.*, outreach – are needed. As for setting priorities, he thought that astronomy was a good example of a community setting its priorities. The chemistry community needs to be mobilized to begin setting its priorities.

Silbey concluded his presentation of the report by presenting three examples of CHE awards demonstrating CHE's interest in supporting future of chemistry and education. The first showed how theoretical chemists are providing software (<a href="mailto:folding@home">folding@home</a>) to the public at large to be able to "play" with molecular chemistry. The second example concerned cutting-edge research of a Nobel Laureate supported by CHE, and the third was about a REU-site which has developed courses to engage undergraduate students in nanoscience.

In the discussion that followed Silbey's presentation, there was concern by the MPSAC on how to address the high workload issue of the division. A suggestion was made that it might be useful to have a set of proposal deadlines staggered by areas *e.g.*, organic chemistry, physical chemistry, *etc.* that would level the workload throughout the year. Turner commented that there was a need for more program directors. Panel reviews were being increasingly used throughout NSF, but since is a panel of experts may not have the expertise for every proposal, *ad-hoc* reviews were still needed. While staggering proposal submission windows would level submissions by subject areas, one would still have peak submission periods at the end of the proposal submission window. It was concluded that there is no ideal solution for this issue.

Members of the MPSAC expressed concern about support for new faculty members, and the discussion turned to the NSF CAREER awards. The success rate for these awards is about 25-30%, and the award itself is amount is for \$90,000 per year for five years. Although the majority of young principal investigators submit proposals under the CAREER competition, there is no restriction for them to do only this. It was also pointed out that the start-up package for new faculty at universities, which has been substantial in the recent years, takes account of the two to three years often takes a new faculty member to obtain external support.

With respect to support of research at undergraduate institutions (RUI), the general tenor was that a collaborative mode was often the best way for support of this type. A large number of RUI awards involved minority research institutions (MRI). The MPSAC felt that a list of awards according to the program that supported these awards, *i.e.* CAREER, RUI, MRI, as well as the type of institution to which the award was made (2-year/4-year colleges, large universities, *etc.*) would be useful. Although such information is already available at the NSF website, an MPS-wide compilation of these statistics would be useful for the MPSAC to have before the next meeting.

The discussion turned to the NIH/NSF cooperative activities. There is now an announcement for proposals to be jointly funded by the two agencies. The MPSAC felt that while closer coordination between the agencies is welcome, a balance is needed between what is conventional chemistry and the emerging thrust (or excitement) in chemistry related to biology. The general consensus was that a cautious approach, which spells out clearly the roles of each agency, would be the right way to go. Within MPS, the Division of Astronomical Sciences has coordinated its activities with NASA, and the roles of the two agencies are clear.

#### Acceptance of the Committee of Visitors Report for the Division of Chemistry by the MPSAC

The members of the MPSAC unanimously accepted the COV report. An acceptance letter would be sent to the Assistant Director of MPS by the Chair of the MPSAC (see Appendix IV). The MPSAC thanked Dr. Silbey for his work in chairing the CHE COV.

#### Meeting of the MPSAC with NSF Acting Director Arden Bement

The Acting Director of the National Science Foundation, Dr. Arden Bement joined the MPSAC session and Pemberton invited the Acting Director to make some remarks.

Bement began his remarks with statements concerning NSF's budgets. He said that NSF is far below the budget authorization pathway but that the FY 2005 budget request currently before Congress may be better than the FY 2006 NSF is preparing for OMB. This was due to the mounting pressures on the budget from the existing deficit. With respect to NSF, Congress is still concerned about transparency in the Major Research Equipment and Facility Construction (MREFC) process. With respect to FY 2006, NSF priorities include protecting the core, broadening participation at all levels, and support of mid-scale projects. There are no new priority areas planned for FY 2006.

In response to questions and comments from MPS/AC members, Bement noted that NSF is working to increase its program staff and to simplify the work of program officers. Both he and the National Science Board (NSB) agree that NSF should adopt criteria, improve transparency, and develop a plan for MREFC projects consistent with recommendations of the Brinkman Report. Furthermore, NSF plans to look at the totality of costs for major new projects prior to starting a project. Furthermore, prior to initiation of any major project, he expected the parent advisory committee to have expressed its support for the proposed project and for the Deputy Director for Large Facility Projects to certify the readiness of the project. Cyberinfrastructure activities will be tailored to the needs of the various sciences, and several workforce development issues are getting attention such as visas for foreign students, retention of students in the pipeline and diversity.

Pemberton thanked Bement for his comments and the discussion.

At this point, the MPSAC was prepared to hear the report of the Committee of Visitors for the Division of Mathematical Sciences. However, while technical difficulties that arose in presenting the report were being dealt with, the MPSAC turned to a discussion of other topics such as the support of theory within MPS, and the Division of Astronomical Sciences breakout group report.

#### Support of Theory Within MPS

This discussion was led by Appelquist, who pointed out that there are a number of issues that need to be discussed concerning the support of theoretical research within MPS and he asked Turner to provide the background on this matter. Turner confirmed that he was concerned about the support of theory within MPS and suggested it might be useful to have a workshop to address common themes for the future of theory support within the directorate. He commented that the line between theory and experiment is somewhat blurred, *e.g.* there were "house theorists" for the ATLAS and CMS experiments, but it is was also important to have some theorists think about ideas and topics not connected to specific experiments. He wondered if there was a problem with the peer review of proposals that involved theory. After some discussion, it was agreed that a workshop on the support of theory within MPS would be a good idea and that a subcommittee of the MPSAC chaired by Appelquist would draw up a plan for a workshop to be held in the fall, 2004. This committee would make an interim electronic report by August 1.

#### Members Retiring from MPS/AC

Turner thanked the MPS/AC members whose terms will expire on September 30, 2004. (Pemberton, Appelquist, Blandford, Hilborn, Pulleyblank, and Salah). He invited MPSAC members to send suggestions and nominations for new members.

#### Long Range Planning: Reports from Divisional Meetings (continued)

Division of Astronomical Sciences (AST)

Salah reported on the AST breakout session. He noted that Sanders attended the AST breakout session for the first time because he has now moved from being associated with the LIGO project (supported in the Division of Physics) to the Thirty Meter Telescope (TMT) project. Salah commented that pressure was still high on AST programs and is expected to go higher due to redirection of NASA [*i.e.* the pending Hubble Space Telescope (HST) closure] programs. Key challenges and issues for AST are: support of the core, mid-scale instrumentation, AST initiatives such as the ATST (which is ready to proceed), and the GSMT and LSST projects. The GSMT and LSST are ready for major R&D efforts. The theory underpinnings to these projects are important, and cyberinfrastructure, especially data archiving, is very important for AST. The breakout group felt that cyberscience funding should reside within individual divisions and that workforce issues need more attention. The implementation plan for the recommendations of the decadal survey still needs to be prepared.

#### Committee of Visitors Report on the Division of Mathematical Science (DMS)

Morrison presented the report of the DMS COV on behalf of its Chair, Dr. Robert Zimmer, Provost, Brown University.

The DMS COV met at NSF, February 11-13, 2004 to review actions taken in FY 2001 through FY 2003. The COV's underlying assumptions were that:

- i) The nation needs a strong program in mathematical research;
- ii) Expanded connections between mathematics and other areas are desirable; and
- iii) Expansion of the workforce and its diversity are important.

Mathematics research in the United States is supported almost exclusively by NSF/DMS. The COV's broad conclusion is that DMS is attentive to all three domains mentioned above. There is a strategic focus on new modes of support, *e.g.* Focused Research Groups (FRG), connections to other NSF areas, and to the Vertical Integration of Graduate Research and Education (VIGRE). The COV examined the balance among individual principal investigator awards and more focused efforts and noted that this requires on-going attention. The COV was enthusiastic about the attention the VIGRE program directs toward workforce issues. The COV highlighted the positive effects of institutes while still calling attention to concerns about the increased number of institutes, the balance of topics within institutes, and the need for evaluation of the effectiveness of institutes. The COV called the attention of NSF to the need for an excellent staff within DMS and for balance among "rotators" and permanent staff.

Morrison noted that the COV performs both an audit function and a strategic function. The COV suggested that additional background material be sent in advance to future COVs.

In responding to the core questions within the reporting template, the COV found that "in general the (DMS) processes are highly effective with appropriate outcomes." There was some concern about the community's understanding of the "broader impacts" criterion and the COV encouraged DMS to work with the community to improve their understanding of this criterion.

#### Acceptance of the Committee of Visitors Report for the Division of Mathematical Sciences by the MPSAC

After a brief discussion, the MPS/AC unanimously accepted the report for forwarding to NSF. The Chair of the MPSAC would send a letter to the Assistant Director of MPS (see Appendix V).

The meeting was then adjourned for lunch.

#### Friday, April 23, 2004

Afternoon Session

The meeting of the MPSAC reconvened at 12:15 P.M.

#### Long Range Planning: Reports from Divisional Meetings (continued)

Division of Mathematical Sciences (DMS)

Pulleyblank reported on the DMS breakout session. The group was impressed by the depth and breadth of programs funded through DMS. It noted that there was a migration of the core to reflect new areas of research. Several breakthroughs were discussed, breakthroughs that warranted New York Times publicity. The group also discussed cyberinfrastructure/cyberscience (CI/CS) issues for the mathematical sciences. Traditionally, mathematicians haven't looked toward computers to advance their work. But the breakout group recognized two areas of mathematics involvement in CI/CS. These were mathematics activities driven by CS (*e.g.*, properties of internet-scale graphs) and mathematics as a component of other sciences such as how does mathematics deal with large data sets (compression; basis functions), the need for computer codes that embody new algorithms,

and mathematicians' service as members of interdisciplinary teams. It was noted that DARPA is beginning to fund fundamental research in mathematics.

Mathematics science priority areas were discussed. There was a suggestion for having postdocs come in and spend a year at NSF, spending 50% of their time on their individual research and the other 50% in a form of "apprenticeship" working on DMS activities. There was also a discussion of peer review by panels versus the *ad-hoc* review process. It was felt that perhaps panels weren't quite as good as *ad hoc* reviewing. Nevertheless, panel reviews were more efficient, and due to workload issues, efficiency might be a necessary requirement.

With respect to workforce issues, there was a need for smarter, more efficient ways of implementing some programs. For example, the requirement of oversight for more than forty-five REU students over a summer by a single faculty member represents too much of a burden on the faculty member.

The group also discussed the COV assessment. It felt that the COV provides beneficial audit oversight, and *adhoc* advice on strategic issues. The strategic issues, however, should be addressed more frequently than the 3-year timescale for COV meetings.

Salah asked what postdocs would get out of the apprentice program. Pulleyblank replied that they would be able to do research plus gain insight into the funding process and what makes a good proposal. It would be beneficial to them as they set up their own research program in the future. Turner commented that NSF science assistants serve some of the same purposes as the proposed postdoc apprentices. Also, the most important contribution of COVs is the validation of the peer-review process. Pulleyblank responded that while the audit process is good, the COV also provides valuable focus and scrutiny on the program as a whole. Aizenman commented that the COV feedback process is important, and that OMB consistently ranks highly those government programs with COV oversight.

#### Division of Materials Research (DMR)

Baker reported on the DMR breakout session. With respect to the core, the optimization of unrestricted/unfettered funding flexibility is important (in lieu of defining the core), and one must be careful not to reduce support for the core through new initiatives. There are numerous examples of materials involvement in CI/CS, including quantum information science, interfaces to mid-range facilities (standards for data acquisition), the Center for Quantum Device Technology, the San Diego Supercomputer Center, and others.

On workforce and outreach issues, the group was impressed with the success of the traveling museum exhibition on material science that was targeted to junior high school students. Pulleyblank noted that there had been a 400% increase in attendance to the museum exhibit over the one-year time frame for the exhibit. Connections are also made with local materials researchers so that they can leverage contacts with educators. The DMR Partnership for Research and Engineering for Minorities (PREM) is up and running and there is significant REU/RET involvement. DMR has a program to offer 50/50 funding for marginal proposals that contain substantial involvement by under-represented groups, and there are various programs for black scientists, international collaborations, *etc.* Within DMR, the strategic outcome area of "Tools" involves approximately 20-25% of the DMR budget. The mid-range instrumentation program will include modeling of future operational costs.

Hellman commented that it was important to articulate what the DMR community does because this was needed for the budget justification process. With respect to success rates of proposals within DMR, it is currently between 30-35%. Weber: noted that materials research is a very competitive field. Some of their more intense competitions have a success rate as low as 10%.

#### Planning for FY 2006

Pemberton began the session by asking for feedback concerning the MPS budget. She asked the group whether the budget increases should be spread out evenly across all MPS divisions, or should there be targeted budget increases allocated to divisions or certain program initiatives? One member said that one year to the next does

not require complete equity, but that historical rates of budget increases (over 5 years or so) should be even across the divisions. Pemberton asked MPSAC members what they thought about MPS budget priorities. One member thought that the MPS leadership should be careful in choosing initiatives so that they do not eat away at the core. Another noted that the Physics of the Universe priority is already funded as part of AST and PHY's core program funds. Another example of a research area that has grown beyond the support of program funds is the NSF Nano priority area. However, this initiative has not brought as much money to DMR as the NSF Math priority has to DMS. It was noted that DMR nano money comes from initiative and core funds because of proposal pressure. One member wondered whether mid-scale instrumentation should be considered part of the core. After much discussion about the possibilities of future mid-scale projects, the consensus was that MPS should properly allocate future funds for operating costs of new instrument facilities.

The discussion then turned towards planning for the Fall MPSAC meeting. The breakout sessions with the divisions were positive, and the time spent in breakout should remain at four hours. Also, breakout reports should come before the long-range planning session so that everyone has a broad update on the entire directorate. The November meeting would have initial discussions of the 2007 budget for Congress. In order to have more productive discussions, the MPSAC members needed more information material with more depth, and needed to receive such material well before the meeting. The MPSAC should limit the number of topics at each meeting and have more in-depth discussions of those topics chosen. Pemberton suggested MREFC's as a topic for the November meeting. When considering MREFC's as a topic for the next meeting, there should be a specific goal/outcome of the discussion, and perhaps Turner should provide a charge to the MPSAC. Additionally, as part of the divisional breakout sessions, each group should consider the question, "What does MREFC mean to the division?" Since the MPSAC is now part of the formal process for NSF-approval of funding for MREFC projects, there is a need to outline where the money for operating costs is coming from when the MPSAC certifies the project. Specifically, is the project funded from new money or out of core funds? Someone suggested that NSF's Chief Financial Officer and the Deputy Director for Large Facility Projects be present for the MREFC discussion.

Another topic suggested for concentrated attention at the next meeting was cyberscience. There should be more time spent discussing the Brinkman Report. One member suggested that several MPSAC members review the Brinkman report and consider the issues and recommendations in context of the NSF response due out in September 2004. On the basis of this suggestion, a subcommittee consisting of Gary Sanders and Gene Futrell was created to do this. This subcommittee should stress the importance of oversight of operating funds for facilities.

Pemberton suggested that another half day be added to the MPSAC schedule. For the next meeting, half of the first day would be spent on new member orientation, with the other two and a half days spent on MPSAC activities. When making suggestions for invitations of new MPSAC members, Pemberton asked the current members to consider the distribution of expertise of the current group. The suggestions and invitations should be made without consultation of the divisions.

Judy Sunley thanked all the members and retiring members for contributions to MPSAC and MPS activities in the last year.

#### Action Items and Future Activities

- 1. Reports for each of the divisional subgroup sessions should be sent to Pemberton as soon as possible (see Appendix II).
- 2. Theory Workshop MPSAC members of the subcommittee associated with this workshop were to provide an interim report on this activity by August 1.
- 3. FY 2007 initial discussions MPS was to provide material relevant to these discussions well in advance of the meeting.
- 4. With respect to support of research at undergraduate institutions (RUI), the MPSAC felt that a list of awards according to the program that supported these awards, *i.e.* CAREER, RUI, MRI, as well as the type of institution to which the award was made (2-year/4-year colleges, large universities, *etc.*) would be useful.

#### Minutes of the MPSAC Meeting of April 22-23, 2004

- An MPS-wide compilation of these statistics would be useful for the MPSAC to have before the next meeting.
- 5. The subcommittee reviewing the Brinkman Report on MREFCs and the NSF responses (Sanders and Futrell) was to report their findings at the November 2004 meeting.
- 6. Members were to submit recommendations for new membership on the MPSAC to Turner as soon as possible.

#### Adjournment

The meeting was adjourned at 2:00 p.m.

#### Appendices

#### APPENDIX I

#### **ATTENDEES**

#### MPSAC Members

Thomas Appelquist, Yale University

Shenda Baker, Harvey Mudd College

Roger Blandford, California Institute of Technology

Janet Conrad, Columbia University

Luis Echegoyen, Clemson University

Mostafa El-Sayed, Georgia Institute of Technology

Lucy Fortson, Adler Planetarium and University of Chicago

Jean Futrell, Pacific Northwest National Laboratory

Frances Hellman, University of California, San Diego

Robert Hilborn, Amherst College

John Huchra, Harvard-Smithsonian Center for Astrophysics

Raymond Johnson, University of Maryland

Jon R. Kettenring, Telcordia Technologies

W. Carl Lineberger, University of Colorado

David Morrison, Duke University

Venkatesh Narayanamurti, Harvard University

Claudia Neuhauser, University of Minnesota

Jeanne Pemberton (Committee Chair), University of Arizona

William Pulleyblank, International Business Machines

Joseph Salah, Massachusetts Institute of Technology

Gary Sanders, California Institute of Technology

#### MPSAC Members Absent

Peter Green, University of Texas-Austin

#### MPS Staff

Morris Aizenman, Senior Science Associate, MPS

Adriaan de Graaf, Senior Advisor, MPS

Laura Bautz, Acting Executive Officer, Division of Physics

Donald Burland, Executive Officer, Division of Chemistry

Henry Blount III, Head, Office of Multidisciplinary Activities

Joseph Dehmer, Director Division of Physics

Arthur Ellis, Director, Division of Chemistry

Eileen Friel, Executive Officer, Division of Astronomical Sciences

Adriaan de Graaf, Executive Officer, MPS

Lance Haworth, Executive Officer, Division of Materials Research

Deborah Lockhart, Acting Executive Officer, Division of Mathematical Sciences

William Rundell, Director, Division of Mathematical Sciences

Judith Sunley, Executive Officer, MPS

Michael Turner, Assistant Director, MPS

Thomas Weber, Director, Division of Materials Research

#### Visitors

Arden Bement, Acting Director, NSF

Peter Freeman, Assistant Director, CISE

Robert Silbey, Massachusetts Institute of Technology

Mitch Waldrop, Office of Legislative Affairs, NSF

### **APPENDIX II**

# MPS Advisory Committee Meeting April 22 - 23, 2004

# **Divisional Breakout Group Assignments**

DIVISIONAL ASSIGNMENTS FOR MPSAC MEMBERS								
	AST	PHY	CHE	DMR	DMS			
APPELQUIST (Absent)		R						
BLANDFORD	X							
HILBORN		Х						
PEMBERTON			Х					
PULLEYBLANK					R			
SALAH	R							
BAKER				R				
GREEN (Absent)								
FUTRELL			R					
MORRISON					Х			
NEUHAUSER					Х			
SANDERS	Х							
CONRAD		Х						
ECHEGOYEN			Х					
EL-SAYED			X					
FORTSON	Х							
HELLMAN				Х				
HUCHRA	Х							
JOHNSON					Х			
KETTENRING					Х			
LINEBERGER		Х						
NARAYANAMURTI				Х				

X,R MPSAC members attending Divisional Subgroup Meetings on 04/22/04

R Subgroup CHAIR, MPSAC member who will summarize Divisional meetings activities to MPSAC

# APPENDIX III MPSAC DIVISIONAL BREAKOUT SESSION REPORTS

# Report on MPSAC Breakout Session with Division of Astronomical Sciences (AST) April 22, 2004

Attendees: MPSAC: Roger Blandford, Lucy Fortson, John Huchra, Joseph Salah (reporter), Gary Sanders

The breakout session started with a review by each program officer of on-going activities and plans for the various AST program elements, including research grants and facilities. It is clear that the pressure from the community remains high on the AST program and that the demand far exceeds the available resources both for research support and the development of new facilities. The MPSAC subgroup sensed that the demand on MPS/AST resources may even increase further as support for astronomical research at NASA is impacted by the on-going major redirection of NASA's mission. If the pressure on the individual investigator grants increases through a larger number of proposals from the community without an increase in funds, the success rate for proposals or the size of the awards will decrease, either of which would be damaging. Given this concern, the MPSAC subgroup advises that careful attention be paid to this potentially difficult emerging issue.

This brief report will not summarize the status and plans for the various AST programs, but will focus on some of the key challenges to be met by the AST Division. It will also comment on the initiatives presented to the MPSAC by the MPS AD for the FY06 budgeting preparations.

- 1. Core program: The core program covers both individual investigator grants (15% of total AST budget) and the facilities and other general support. The budget for non-facilities activities in FY04 remained flat or declined, due to specially-directed funds towards facilities. While this special funding was to support certain exigencies at one national facility, its impact was painful and will be very damaging if it continues. The core program remains the highest priority for continued growth and support in AST.
- 2. *Mid-scale projects*: A large number of projects at the mid-scale level remain on the list, and it appears that many of these projects will have to be funded from the AST core since a new funding initiative for mid-scale projects is not expected to be implemented at NSF. It is disappointing that the results of the NSB study on mid-scale facilities and the recommendations of the MPSAC in its previous reports cannot be followed so that the gap between the MREFC and MRI levels of support can be filled. Nonetheless, the MPSAC subgroup was pleased that the newly-launched *'Physics of the Universe'* initiative in MPS allow design studies and technology development for two MREFC-level projects, namely the Giant Segmented Mirror Telescope (GSMT) and the Large-aperture Synoptic Survey Telescope (LSST), to appear in the President's FY05 budget request. Other AST projects at both the MREFC and the mid-scale levels still require the development of an implementation plan that is realistic in terms of its expected funding and that can fulfill the community's expectations.
- 3. MREFC projects: Several AST projects that were highly recommended by the Decadal Survey of Astronomy and Astrophysics are being prepared for implementation. The Advanced Technology Solar Telescope (ATST) project is approaching the end of its funded design and development phase and a proposal for construction as an MREFC project is now under review. As noted above, both the GSMT and the LSST are ready for the design phase as a first step towards the MREFC program. These projects, indicated by the MPS AD in his planning discussion with the MPSAC for potential implementation in FY06, are endorsed by the AST subgroup. The subgroup also recommends that MREFC support of a proposed project should include theory and computation as part of that project. Such theoretical work should be clearly documented in the proposal for the project since it is an important component of the effort, and the rules for MREFC should be re-examined to allow its support. Similarly, operations support should be included in the planning for MREFC funding through the development

of a funding line for the facility operations, since drawing such funds from the core will impact the remainder of the program.

- 4. Cyber-science and infrastructure: The AST program has many applications for cyber-science including the handling and mining of large data bases and the exploitation of high-speed networks. AST projects have been pathfinders in cyber-science and have established standards for common formatting of data and for common data analysis and imaging packages. One area that needs additional attention and support is the archiving of the astronomical data sets in a manner that can preserve their long-term accessibility and utility. Another area of importance is the utilization of professional software personnel in the development of astronomical systems since their expertise can provide an efficient framework for such developments. Two programmatic aspects of cyber-science and infrastructure were identified by the AST subgroup: (a) funds for cyber-science implementation are recommended to be provided to the AST Division (and other MPS divisions) for distribution according to the Division's priorities, and (b) care should be taken in the transition from the Information Technology Program (ITR) to the Cyber-Infrastructure (CI) program since commitments for multi-year ITR grants need to be supported from sources other than the core, and preferably from the CI program itself.
- 5. Workforce: More effort should continue to be applied to retain people in the workforce stream, especially women and under-represented minorities. The AST subgroup discussed the decrease of women in astronomy from the undergraduate levels (roughly 50% in REU site programs) to the graduate and professional level (roughly 15% of the American Astronomical Society (AAS) membership). For minorities, the subgroup discussed the benefits of working at the pre-college levels and of recruiting at community colleges. The AAS needs to be fully engaged in these activities to support the astronomy community in fulfillment of the workforce diversity goals.

# Report on MPSAC Breakout Session with Division of Chemistry (CHE) April 22, 2004

Attendees: MPSAC: Luis Echegoven, Mostafa El-Sayed, Jean Futrell (Reporter), Jeanne Pemberton;

CHE Division: Don Burland, Michael Clarke, Kathy Covert, Art Ellis, Joan Frye, Janice Hicks, Carol Korzeniewski, Bob Kuzckowski, Tyrone Mitchell, Charles Piebel, Celeste

Rohlfing, Brian Tissue

In our general discussion an emerging area of concern, noted in our previous meeting with the Division as a Sub-committee of MPSAC, is the dramatic increase in the fraction of academic chemistry research funded by the NIH as they have experienced a doubling of their research budget. Following the well-established principle of "following the money" more and more chemistry PI's are succeeding in NIH competitions, particularly in the sub-discipline of organic chemistry. The magnitude of funding in individual NIH grants is much larger than in NSF grants, typically \$190K per annum in direct funding and 5 years duration compared with less than \$100K in direct costs and 3 years duration for NSF Division of Chemistry grants. There is accumulating anecdotal but consistent evidence that this trend has unintended consequences in preferential hiring of faculty and preferential deployment of graduate students and postdoctorals in research areas related to NIH mission interests. This is further exacerbated by financial pressures on universities to maximize recovery of indirect costs and recoup startup costs for new faculty.

1. Cyberscience and cyberinfrastructure: With the caveat that our community likely needs further education concerning emerging opportunities, there is consensus among our sub-group that chemical sciences will benefit broadly from deployment of cyberscience tools and development of cyberscience infrastructure in many ways we can anticipate and in ways only vaguely defined. Particular examples are access to rapidly expanding databases that are widely accessible and based on user-friendly formats. The results from a recent NIST/NSF

workshop on creating and curating gas phase kinetics and thermodynamics data sets were reviewed briefly and endorsed as a relevant example. Data mining, modeling, methodology, chemical reactions and reactivity lend themselves to cyberscience approaches. Development of collaboratory tools for remote access to instrumentation, for active collaboration at a distance, and for rapid access to information and data bases is an area that appears ready for exploitation. Creation of virtual reality laboratories as supplements or substitutes for laboratory experience in chemical education appears now to be feasible and may be an attractive means to augment existing pedagogical approaches. This is especially attractive, since it may be extensible to 2-year institutions that are increasingly important contributors to undergraduate chemical education. More effective means for coupling theory, modeling and simulation with experiment and advanced instrumentation are additional plausible examples of cybertools that can benefit the chemistry community. Dealing with fragmentary and dispersed data and with undersampled data are long-standing problems that may also be amenable to cybertool exploitation. A spirited discussion of the possibility of developing "Science@Home" modules analogous to Folding@Home", the website based at Stanford that allows tens of thousands of individuals around the world to contribute to protein folding calculations on their PCs, concluded our discussion of this topic.

We are convinced that this priority area encompasses much of cutting edge research and education in chemistry and that the community needs the opportunity to be both better educated about and stimulated to think more expansively about these possibilities. In this spirit we recommend that a workshop on domain-specific cyberscience and cyberinfrastructure be organized. Among the outcomes of such a workshop may be identification of investments in large, mid-scale (\$2M to \$100M) projects.

2. The Core Program: The imputed skewing of research, education, recruitment of students and faculty related to dramatic increases in the NIH budget was once again discussed in the context of protecting core strengths in chemistry. The dichotomy that a priority emphasis on "Molecular Basis of Life Processes" was enthusiastically endorsed by our group was considered. Although greatly welcomed, the relatively low level of new funding of \$2M in the '05 budget is too small to have much effect on research trends in academic chemistry. However, it can be effectively leveraged by partnership with other agencies such as DOE and NIH and constitute a new priority focus area in chemistry. Focusing on the sequence of molecular interactions and deducing how weak forces mobilize self-assembly is clearly a grand challenge chemical problem for advancing our knowledge of both life processes and nanoscience. Developing the instrumental tools and theoretical models to observe and interpret these processes is a challenge falling squarely in the domain of chemistry. It follows that advancing molecular understanding of life is a priority area that should be emphasized. Accordingly we strongly encourage CHE to continue and expand their dialog with other agencies, notably NIH, to draw their attention to research opportunities at the border of our discipline and explore opportunities for workshops, symposia, joint funding and other mechanisms that pull together research on fundamental research relating to the chemistry of life processes.

One theme that captures many of these ideas is "chemical imaging". The ability to image chemical systems at lateral size scales from microns down to single molecules, and for single molecules or small collections of molecules, to track them in space and time will enable advances on a broad front. We endorse the idea of a workshop, perhaps in partnership with other agencies like DOE and NIH, to explore chemical imaging opportunities with the chemical sciences community. Among the outcomes of such a workshop may be identification of investments in large, mid-scale (\$2M to \$100M) projects.

We also discussed changing the definition of "core research" in the chemical sciences. We applaud the fact that a large fraction of research grants supported by the Division remains in the category of individual investigator grants. This category of grants has traditionally been the definition of core research. It is absolutely essential that support of individual investigator grants be protected and the fraction of grant support within the Division going to this category of research funding should be sustained. However, we feel the time has come to broaden the definition of core research to incorporate exciting science done by more than one investigator and at the interface between disciplines. Our proposed definition is that all research focused on fundamental molecular-level questions is properly included in the core, independent of the number or type of investigators involved. We also recognize that professional chemists are often productively involved in service roles in both teaching and research. Although valuable and appropriate, our opinion is that this kind of research is not part of the core.

When the contribution is intellectual and addresses fundamental chemical questions, it is within the core of our discipline. Core research is broadly but simply framed around advancing molecular understanding. This modification of the concept of core science has the implication that an even larger fraction of CHE support is for core science, which we in fact believe to be true. However a statistic that should be tracked and reported to MPSAC and the community is the fraction of support devoted to single investigator PI grants.

3. Workforce issues: A number of important initiatives aimed at workforce issues currently in progress were briefly reviewed. The Undergraduate Research Center program, the new class of postdoctoral and senior fellowships, the "Discovery Corps", and a possible program for engaging talented high school students in research were described. These programs promote the NSF objective of integrating research and education. We also commend the American Chemical Society's new experiment in faculty recruitment, the Academic Employment Initiative, supported in part by an award from the Division of Chemistry. This initiative provides opportunities for search committees and potential faculty candidates to become acquainted at national American Chemical Society meetings. Our general conclusion is that the Division has been proactive in workforce issues.

#### 4. General Issues:

Engaging the Community: The chemical sciences community is broad and has been described as individual entrepreneurs that have no generally accepted means for reaching consensus and setting priorities for the field. The Chemistry Division is increasingly recognized as leading the evolution of the discipline. This can and should be expanded and the MPSAC chemists are willing to help in this endeavor, possibly by organizing a forum at a future ACS meeting that includes MPSAC members and explicitly challenges the community to examine new opportunities and challenges in chemistry. Workshops have emerged as an important tool for this ongoing education effort and we discussed ways of both enhancing the role of workshops and distributing the outcomes of such workshops in the form of workshop reports more broadly. A recommendation was made that these reports should be retained for several years and that access be simple, convenient, and prominently featured in the Division web page. One idea discussed was out-sourcing of workshop reports to a commercial, web-based archiving service with discipline-specific links contained on the appropriate NSF web pages. Given the relatively minor expenses associated with such services, our sub-group felt that this could be a very effective and accessible means of archiving and distributing such reports.

Department chairs were identified as a very important node both for disseminating this information and for broadening the dialog on priorities in chemistry. Current focus issues include cyberscience and mid-range instrumentation. One or more C&E News editorials were mentioned as one means for calling attention to the need for setting priorities.

A particular outreach effort crystallized at our meeting was organizing a workshop to showcase broader impact (Criterion 2 by which NSF proposals are evaluated) success stories at a national ACS meeting. Luis Echegoyen volunteered to organize this workshop, most likely as a poster session for best practices. "Nuggets" emerging from this workshop will be collected and posted on the web, to help educate the community in this area. As noted in the Division of Chemistry 2004 COV report, it is also important to educate CAREER award proposers on what types of projects might be included in the education section of their proposals. The workshop might be set up to include these examples, as well.

Concluding Remarks: Chemistry MPSAC members who have attended previous MPSAC meetings found this to be the most productive breakout session in our experience.. This reflects, in part, the extended time of 4 hours and the structured agenda of questions to be addressed. However, it is our opinion that the special meeting of MPSAC chemists with the Division in March is a major factor in the success of this breakout session in that it provided a foundation on which to develop cooperative creative thinking. These extended interaction s gave us better understanding of how the Division operates, increased trust and comfort level between ourselves and program officers, and led to a synergistic mode of working together that was immediately apparent in our session. Jeanne Pemberton described it as a "bonding" experience that goes beyond our frequent reference to chemical bonds.

# Report on MPSAC Breakout Session with Division of Materials Research (DMR) April 22, 2004

Attendees: MPSAC: Shenda Baker, Frances Hellman and Venky Narayanamurti

- 1. *Core Program:* What does the materials research community mean when it talks about protecting the core? What are the implications for DMR?
  - a. A number of different interpretations were expressed, but in the end, the exact definition may not be as important as protecting the ability to optimize the unrestricted or unfenced funding in order to maintain flexibility. With less restricted funds, DMR can continue to fund the most exciting, high quality proposals in the core disciplines and to push the boundaries of the fields in materials science and engineering.
  - b. The core programs in DMR can be found in a variety of programs or topical groupings such as "condensed matter physics", "metals, ceramics and electronic materials", "solid state chemistry and polymers", and "materials theory". Many core activities are funded through the MRSEC's and cofunding in STC's and NSEC's, whether the funding is intiative based or programmatic. In addition, support for the core activities is found in the instrumentation opportunities of National facilities and instrumentation such as IMR, MRI and mid-range instrumentation.
  - c. One note to keep in mind that if "the pie" does not get bigger in years where new initiatives are created, it is not acceptable to keep taxing the core until core disappears!?
  - d. We note that, the funding in DMR increased by less than 1% last year. although DMR has significant investments in the new initiatives such as Nano and Mid-range instrumentation. As DMR will play a significant role in Cyberscience, we hope that attention will be given to looking at the relative historical trends among the divisions with respect to funding these initiatives and to make sure that DMR is not missing important opportunities due to limited funds.
- 2. Cyberscience and Cyberinfrastructure: What are the strongest drivers for materials research toward expanded participation in cyberscience and use or development of cyberinfrastructure? What are the implications to DMR?
  - a. DMR already has a substantial role in ITR with a current budget of about \$10M. Quantum Information Sciences (QIS) is a large component, but is funded by DMR programmatic sources. 45 ITR proposals were identified as DMR related this last year. Also DMR supports hardware aspects such as spin electronics, superconducting electronics, Josephson junctions, etc. and a number of efforts in materials science (spin systems, quantum computing, electronic materials and photonics, etc) that will produce the next generation of computers.
  - b. DMR has a Materials Theory program (which includes Condensed Matter Theory) which is developing tools to make the connections across length and timescales (the atomistic to macrosopic properties). These will continue to be a motivating force and key to breakthroughs for many researchers in DMR.
  - c. CI/CS is and will continue to be essential in DMR in activities including theory, development of algorithms and software, data collection, analysis, interfaces and visualization at major facilities, international activities, data archiving and visualization.
  - d. Some CI/CS impacts will be broader and have community developed standards (like neutron/x-ray

scattering communities, GSAS codes for diffraction analysis) some will be more localized like local algorithms specific to group architechtures, specific research questions and prioritization is best done by

the community and within the division.

e. DMR will continue to contribute in a meaningful way to development of algorithms, codes, data archiving, visualization as is necessary to support the science and engineers such as Center for Quantum

Device Technology at Clarkson, Center for Theoretical biological Physics at UCSD (Scripps, Salk institute and Sand Diego Supercomputer Center), Institute for the Theory of Advanced Materials in Information Technology, U Minn and Information Technology Research: Modeling and Simulations of Quantum Phenomena in Semiconductor Structure of Reduced Dimensions centered at GaTech.

- 3. *Workforce:* What are the most pressing issues for materials research with respect to developing the workforce and broadening participation in the field? What are the implications for DMR?
  - a. DMR is making significant investments in the Workforce of the future. The division recognizes that they
    - need to provide opportunities to a broad group of people in order to ensure the strength of the field in the future.
  - b. DMR has participated indirectly in "strange matter", a traveling museum exhibition targeted to 5<sup>th</sup>-8<sup>th</sup> graders by providing scientific input through the MRSEC's. This exhibition has been tremendously successful so far at the Liberty Science Center in New Jersey (attendance is over 400% greater than last year at this time) and the National Atomic Museum in New Mexico. The associated web site highlights a number of NSF funded materials scientists as well at www.strangematterexhibit.com
  - c. PREM (Partnership for Research and Engineering for Minorities) was initiated by DMR.
  - d. DMR invests regularly in REU's and RET's.
  - e. For high quality proposals at the borderline between funding and not, the division has worked to increase participation of women and minorities by using Division Directors funding to match the Program Directors by 50%.
  - f. DMR has supported meetings of the National Society for Black Physicists sponsor meetings where students give research presentations, but also learn about careers in physics from graduate students and faculty.
  - g. DMR continues to invest in international programs (Europe, Americas, Africa and Asia).
  - h. DMR might consider how to encourage re-initiation grants through ADVANCE and SGER that would facilitate materials scientists and engineers who have left the workforce finding their way back onto the "pathway" (rather than back into the "pipeline".
  - i. Funding trends for women and minorities in DMR reflect the demographic distribution of women and minorities currently in DMR fields. Note that engineering and physics has typically very low participation by women and non Asian minorities.
- 4. Tools for materials research and education:
  - a. DMR has a large investment in the tools required by materials scientists and engineers, mid-range instrumentation, IMR, MRI and user facilities (NAF) which is about 20-25% of DMR budget over the past 10 yrs. Given the nature of materials science and engineering, such an investment is important and expected.

- b. Energy recovery linac (ERL) currently being jointly considered with PHYS) is an interesting potential MREFC that is pushing the envelope in coherent X-ray production. Currently at the stage of proof of principle, if successful, any number of linac's could be retrofitted to produce powerful (parasitic) coherent X-ray sources.
- c. DMR has a well-developed model for addressing sustained support of mid-range instrumentation. Given

the nature of the instruments typically funded by DMR (leveraging off of huge investments by DOE), each proposal must have a well-developed plan in place for identifying operations, maintenance and support before an instrument is funded to be built. It may be that the instrument is subsequently supported by the facility at which it is built or by NSF, but it must be determined up front.

- 5. Emerging areas and opportunities in materials research: DMR makes contributions in a number of areas identified by NSF as emerging areas. Not only does the science address "Creating the molecules and materials that will transform the 21<sup>st</sup> century", but also the other categories of science "themes" addressed at the meeting. DMR will continue to lead in cross cutting activities in areas such as
  - a. imaging materials in 3D at the atomic scale and at the nanosecond time scale
  - b. designing and creating materials by learning from nature
  - c. bridging across length and time scales from atoms and molecules to complex structure and devices
  - d. looking for new, undiscovered phases of matter
  - e. understanding and using biological self-assembly
  - f. designing and producing a solid-state quantum computer
  - g. enabling better public understanding of science
  - h. developing the fundamental understanding to move from a fossil-fuel-based economy to a sustainable one

We applaud DMR for developing the "Big Questions" and core research ideas. Some of the specific questions on the DMR proposed questions are:

#### Big Questions on creating the molecules and materials that will transform the 21st century:

We wonder if there could/should be more on fundamental science here, not just plans about useful materials. For example,

- 1) Can we create new classes of scientifically important or technologically useful materials that don't presently exist?
- Can we design and produce functional molecules and materials for a chosen scientific goal or

chosen application?

- 3) Understanding weak molecular interactions seems to us needs a "why" e.g. which control.....
- 4) Understanding and controlling high Tc should be in this section, not under the foundation for health, prosperity, security. It is not obviously relevant to these, and is certainly less relevant than e.g. understanding issues in magnetism, which do not appear in this list but probably should.

#### **Big Questions on Developing Tools:**

Time domain tools should be added

Big Questions on conducting basic research that provides the foundation for our national health, prosperity and security:

- 1) Can we develop new materials or new approaches that allow the explosion in computational power and memory to continue (i.e. Moore's law)?
- 2) Can we develop new cheap nano-sensors and massive data analysis and transmission requirements that allow us to monitor and predict environmental problems ranging from pollution to flooding to tornadoes to traffic flow?

#### 6. General Issues:

#### Organization and support for condensed matter physics:

There is concern in the community that fundamental CMP (both experiment and theory) is not getting the support it should, due to an excess emphasis on applications. It is not clear that this perception is based in reality of funding distributions within DMR. Both CMP and MT (materials theory) do include a large number of undeniably fundamental physics grants. Funding decisions for individual grants are based on a peer review system which sets priorities according to the community finds important; this system which relies on near unanimous agreement due to the low funding % probably does not favor far reaching speculative fundamental physics, an NSF-wide issue. This has been presented as a "theorist" issue, but is broader than just theory - it is difficult to use the peer review system to properly assess speculative proposals since inevitably some reviewers will rate them as unlikely to succeed, and indeed high risk means only a few will succeed.

DMR with help from MPSAC subcommittee members have completed a "Dear Colleague" letter to help ensure that the community correctly views criteria 2 in the broad way it is intended, not solely as applications to technology or K-12 outreach, but the full breadth of possible broader impact.

We note that CMP has had the lowest increase in funding of any of the sub-divisions in DMR, and that many outstanding proposals have to be turned down each year. This is not unique to CMP, but given the rate of growth of CMP graduate students and PI's, may perhaps be worse here.

MPS should work harder to include fundamental CMP breakthroughs in their public statements of "Physics breakthroughs" in order to reduce some of the most strident criticisms from the CMP community. Not all Physics breakthroughs are funded by the Physics division of MPS. Likewise, DMR has agreed to provide nuggets to PHY for them to disseminate.

A sub-committee to address the theory portion of this issue and perhaps develop a workshop was proposed by MT to the full MPSAC and will proceed (includes Tom Applequist, Venky, FH).

# Report on MPSAC Breakout Session with Division of Mathematical Sciences (DMS) April 22, 2004

Attendees: MPSAC: Raymond Johnson, Jon Kettenring, David Morrison, Bill Pulleyblank (Reporter)

- 1. Cyberscience/cyberinfrastructure: The mathematical sciences will have two complementary roles to play:
  - a) Contributions by the mathematical sciences will be a key part of many tools for cyberscience. These will come from new algorithms, new mathematical models and new methods for analyzing the massive amounts of data being collected. These advances will form key parts of the new, computer based tools for cyberscience which will exploit the capabilities of the cyberinfrastructure.

b) Models that exploit the emerging cyberinfrastructure are becoming an increasingly important part of a mathematical scientist's tools. These enable experimentation which can form the basis for discovery of phenomena and the resultant development of theory. Computational results often provide a proof point for mathematical theory.

One problem that will have to be solved is the creation of sources of funding for this research. The ITR initiative will be finished at the end of 2004 and the funding administered by CISE for funding cyberinfrastructure is being focused on the infrastructure itself, rather than on the tools that will take advantage of it to solve the problems of other areas of science. If these funds come from DMS (or MPS) it will create a requirement for new funds, at the expense of other programs.

We are seeing many examples of massive datasets being collected. Sometimes these are numeric, such as readings from radio telescopes, networks of sensors, or transactions on the world's financial markets. But many others are noncoded data, such as audio streams or visual images. These require new methods to approximate and analyze this data. In addition, some of these data files are based on non-physical data and may require the development of new methods to model.

Two areas that we believe will be key are statistics and data mining. The former focuses on developing statistically sound models and estimating their associated parameters in order to determine the properties of large data sets.. The latter, traditionally more computational in nature, focuses on algorithms that can identify "unexpected" or "unusual" events occurring in large datasets, which enable detection of anomalies. This is closely related to the area of model-based detection in statistics.

Finally, we point out that there are two types of large datasets: *Repository* datasets contain data that has been collected and made available, frequently in the form of databases or data warehouses. Most traditional data analysis and statistics have focused on this type of data. *Streaming* data is usually sensor generated and consists of continually increasing amounts of data which must be analyzed, and often summarized in real time. The understanding and modeling of these types of data sources require new methods to be developed.

2. Living with the Mathematical Sciences Priority Area: The increased funding provided by the MS Priority area is providing an excellent opportunity to increase the amount of research being carried out, particularly research focusing on interactions between the mathematical sciences and other areas of science and engineering. We feel that overall the DMS has done an outstanding job of initiating programs in this area which are already showing signs of success. These programs generally are supported both by DMS and some other funding agency.

This is creating a real risk that there will be insufficient funds in the future to support the core research in the mathematical sciences. There is often considerable debate as to what constitutes the "core", but it probably can be viewed as the study of mathematics for its own sake, rather than for its relevance to other disciplines. The history of the mathematical sciences contains many examples of core discoveries that have subsequently proven to have important uses, and there is general agreement that this type of research should not be reduced, particularly because NSF is often the only agency funding much of it.

The challenge this presents is to continue to grow the interdisciplinary and applied programs while continuing this basic support. It is made particularly difficult because there is a goal of increasing the size of core grants as well as their duration. If this takes place, there will have to be a decrease in coverage.

#### 3. General Discussion:

#### **Mathematical Sciences Institutes:**

These continue to thrive and to be an important part of the US and global mathematical sciences enterprise. The institutes all have different roles and characteristics and do seem to be an effective way of accelerating development in new areas as well as continuing development of core areas.

These also provide a means for training new members of the Math. Sciences community, such as postdoctoral fellows, as well as bringing together mathematical scientist and researchers from other areas to enhance collaboration.

However, in the face of increasing pressure for funding, we do see a risk that these will come under pressure. We encourage these institutes to seek to develop alternate sources of support which will complement the funds provided by NSF. This is being done to a good degree by the IMA and should be part of the plans of other institutes, as funding opportunities arise. This can be a time to be creative!

#### **REU Program:**

The REU program is a very effective way of introducing undergraduates to research, but it is typically very labor intensive for the mathematical scientists who run the programs. It would be desirable to have more efficient ways of accomplishing similar goals. Some initial experiments with undergraduate summer institutes focusing on solving of industrial programs have shown potential.

#### **DMS Staffing Issues:**

The DMS is facing severe staffing problems. The establishment and management of interdisciplinary programs are very demanding of time and the number of applications for funding support in all programs continues to increase. This is putting an increasing demand on program officers, with the result that they have virtually no time for the participation in conferences and academic visits essential for them to do their jobs well.

The problem is not just obtaining the authority to hire additional staff, but also in locating suitable people for these positions. Rotators are an essential component of this work force, but they require time to become effective, and often are unwilling to commit to terms longer than a single year. Often a two year rotation would be preferable, because of the learning taking place during the first year.

We believe that appropriate assistants could ease the burden on program officers. The understanding of the operations of funding programs and the criteria for success could be an important part of the education of young researchers, if an appropriate mechanism can be developed for including them in the process.

#### **DMS COV Report:**

The COVs provide two types of value: they audit the effectiveness of programs and they provide input on a range of *ad hoc* issues. It could be of value to DMS to have access to these types of groups more frequently than just every three years. The MPSAC does provide this function to a limited degree, but only contains four members, so is too small to be effective in this capacity.

Overall, we were impressed with the quality and breadth of the DMS Research program, and congratulate Bill Rundell and his staff on their effectiveness in launching a broad set of activities as part of the Mathematical Sciences Priority Area.

Report on MPSAC Breakout Session with Division of Physics (PHY) April 22, 2004 Attendees: MPSAC: Tom Applequist, Robert Hilborn, Janet Conrad, Carl Lineberger

1. *General issues:* Joe Dehmer began by noting that the budget of the Physics Division, \$228M in FY 04, breaks down along the following lines: approximately 50% for core support of PI's, approximately 33% for facility operations, and 15-20% for the support of Centers.

There are now 13 Physics Frontier Centers, with the next proposals due in August of 2005. The Division anticipates being able to support two new, "medium size" Centers in each subsequent funding cycle.

On facilities support, Dehmer stressed that the current commitment to the Cornell accelerator runs through FY08, and that, as "sole owner" of LIGO, the Physics Division feels a strong commitment to fund its upgrade. He projected that IF the budget of the Division increases by at least 3% per year over the next few years, all facility-support commitments can be met. These do not include the Large Hadron Collider and the possible Underground Laboratory.

Dehmer stressed that the 50% allocation to PI support in the Division is a judgement call that should always be re-assessed. Restricted to this level, it has created a high degree of stress, especially on theory grants. There is currently about \$20M per year devoted to core support of theorists, excluding Centers such as the Kavli Institute for Theoretical Physics. There are many accomplished young theorists with little or no support, and lots of bright students who cannot be supported.

The FY05 budget request of \$236M for the Division, benefiting from the Physics of the Universe initiative, is good news for the Physics Division. But given the current budget climate in Washington, Jow Dehmer is only "cautiously optimistic" about future years.

We discussed the Rare Symmetry Violating Processes (RSVP) MREFC, beginning with a brief update of the initiating years FY99-FY04. After much delay within the Foundation, RSVP seems to be on track. Following a \$6M start in FY04, it is slated for \$30M in the FY05 budget. Also, a director, Bill Willis of Columbia University, has been appointed. This program is very exciting scientifically, and the Directorate and the Physics Division must to do all they can to keep it on track.

At this point, we were joined by Michael Turner, who reviewed the reasons for the disappointing FY04 budget of \$228M for the Physics Division. He stressed the difficulties leading to the small increase relative to the FY03 budget of \$224M. Across the Directorate, he had to work within the overall Presidential budget, follow the various directives that came from Congress, and support the core programs at adequate levels. Michael pointed out that this budget was especially hard on facilities operations. In this area, he stressed the importance of "appetite control", the importance of being able to support operations for any new facility being put forward.

After Michael left, we turned to a discussion of the proposed Underground Laboratory. There is much exciting science to be done here across a range of fields including physics, geology, biology, and astronomy. Joe stressed that the necessary operations support for this laboratory cannot come from the Physics Division budget within the scenario of 3% increases per year. It is very important that the Physics Division and the MPS directorate consider the budgetary aspects of this project carefully and insure that the peer review process remains at the forefront as the project is considered further.

- 2. Cyberscience/Cyberinfrastructure initiative: It was pointed out that the Physics Division, together with the CIS Directorate, has played a leading role in the development of the Data Grid. Joe said that he could foresee \$7-9M being available for this initiative in the FY06 budget. There was a strong feeling among the Physics Division staff members that funds within this initiative should be invested from within the divisions by the program directors. They are the "support professionals" for both large- and medium-scale projects.
- 3. Workforce and education outreach issues: These were discussed at some length. Marvin Goldberg described the success of Quark Net as well as other education and outreach activities associated with the LHC and RSVP. There are currently about 50 REU sites supported by the Division, some of which include RET programs as well. We discussed the education activities of the PFC at Hampton University, and Joe noted that a

#### Minutes of the MPSAC Meeting of April 22-23, 2004

Physics Education Research Grant at a yet-to-be announced institution has been approved for FY05. There was general sense that the Physics Division has been very successful in education and outreach. It will be very important in the future, however, to develop some agreed-upon metrics for the measurement of success in these areas.

4. *Mid-scale instrumentation:* These are projects in the \$10 - 50M range. These are extremely important in high energy physics for example, since the NSF is a major source of support for projects in this range. The Physics Division and the MPS Directorate will need to develop mechanisms for the prioritization of these projects.

The MPSAC members of this breakout session thank Joe Dehmer and the members of the Physics Division staff for the time they devoted to this breakout session, and for their thorough and candid discussion of the Division activities.

# APPENDIX IV THE UNIVERSITY OF ARIZONA TUCSON ARIZONA

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June 24, 2004

Dr. Michael S. Turner, Assistant Director Directorate for Mathematical and Physical Sciences National Science Foundation 4201 Wilson Boulevard Arlington, VA 22230

#### Dear Michael:

I am pleased to inform you of the formal acceptance of the Report of the Committee of Visitors (COV) for the Division of Chemistry (CHE). Dr. Robert Silbey, Chair of the COV, presented the Report to the MPS Advisory Committee (MPSAC) at its April 22-23, 2004 meeting. The Report was laudatory regarding the effectiveness of the Chemistry Division both in facilitating scientific discovery in chemistry and related areas as well as in the administration of the grant proposal review process. The need for a strong emphasis on single investigator grants that has characterized past CHE funding was noted. The positive impact on the community of CHE funding for instrumentation, especially instrumentation funding for undergraduate institutions, was also noted.

The COV report noted several important issues and opportunities that the MPSAC believes should receive attention. Specifically, the COV noted "the increasing disparity between the average size and duration of individual investigator awards from the NIH and NSF." Concern was expressed that "not only is this disparity driving excellent science out of the NSF portfolio, federally funded chemists are increasingly redirecting their research towards medically-related areas. If this trend continues, critical areas of national need (e.g., chemical and biological sensors, instrumentation), scientific infrastructure and workforce training will be underserved." Although the Division has begun efforts to increase grant duration as a partial solution to this problem, the fundamental limitations imposed by the Divisional budget preclude resolution of this problem in a substantial way. The potential deleterious long-term impact on the discipline resulting from this disparity cannot be overstated.

The COV also commented on the problems of the staff workload imbalance created with a finite proposal submission window, and the need for continued education of the community about the "Broader Impact" criterion for proposal evaluation. With respect to the latter,

although CHE has been a leader within MPS in communicating with the community through its "Dear Colleague" letter of 2002, the COV noted the variability in attention to this criterion in proposal reviews. Thus, the MPSAC encourages the Division to continue its efforts to educate and engage the community on this issue.

Finally, the COV encouraged the Division to "energize the community to take part in the nascent NSF programs in cyber-technology" since "chemistry ought to be a major player in this effort because of [its] strengths in molecular level computation." The MPSAC concurs with this directive.

We are grateful to the COV and its Chair for the excellent, in-depth review of the Chemistry Division, and to the Chemistry Division staff for their thorough preparations for this COV review and for their commendable work.

Sincerely,

Jeanne E. Pemberton

Chair, MPS Advisory Committee

cc: R. Silbey, A.B. Ellis, M. Aizenman

# APPENDIX V THE UNIVERSITY OF ARIZONA TUCSON ÁRIZONA

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June 24, 2004

Dr. Michael S. Turner, Assistant Director Directorate for Mathematical and Physical Sciences National Science Foundation 4201 Wilson Boulevard Arlington, VA 22230

#### Dear Michael:

I am pleased to inform you of the formal acceptance of the Report of the Committee of Visitors (COV) for the Division of Mathematical Sciences (DMS). Dr. David Morrison of the MPS Advisory Committee (MPSAC), and a member of the DMS COV, presented the Report to the MPSAC at its April 22-23, 2004 meeting in the absence of Dr. Robert J. Zimmer, Chair of the COV. The Report strongly endorsed the work of the Division of Mathematical Sciences and enthusiastically noted the enhanced strategic focus of DMS in the three major domains of: 1) continued and expanded strength of the nation in core mathematical sciences research, 2) continued and expanded strength in connecting mathematical sciences to other areas of natural science, technology, and social science, and 3) expansion of the workforce in the mathematical sciences. The Report cites the "boldness and imagination" of DMS in "vigorously and successfully [addressing these] major strategic issues" and expressed "broad enthusiasm and appreciation for the innovative work and productive flexibility of DMS."

The Report articulates several issues that the MPSAC believes should receive attention. Specifically, the COV suggested that DMS develop a formal assessment plan for the effectiveness of the VIGRE program in light of the significant commitment of resources that this program commands. In addition, in light of the increasing support of and role of institutes in the DMS portfolio, the COV questioned whether other programs supporting conference activities are now somewhat redundant and whether certain areas of core mathematics are adequately represented in the institute portfolio. The MPSAC recommends that these questions be carefully considered by DMS as it implements its vision for future activities.

Finally, the COV Report indicated that there is "considerable uncertainty within the community about what constitutes an adequate response" to the "Broader Impact" criterion. The COV Report suggests greater community education on this issue and further recommends that "DMS immediately begin work with the community to accelerate this process, and be as explicit as possible about the

appropriate interpretation of 'broader impact' for various types of proposals." The MPSAC strongly endorses actions to educate and engage the community on this issue.

We are grateful to the COV and its Chair for the excellent, in-depth review of the Division of Mathematical Sciences, and to the DMS staff for their thorough preparations for this COV review and for their commendable work.

Sincerely,

Jeanne E. Pemberton

Chair, MPS Advisory Committee

cc: R.J. Zimmer, W. Rundell, M. Aizenman

#### APPENDIX VII

### Certification of Accuracy of Minutes of April 2004 MPSAC Meeting



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July 12, 2004

Dr. Michael S. Turner, Assistant Director Directorate for Mathematical and Physical Sciences National Science Foundation 4201 Wilson Boulevard Arlington, VA 22230

#### Dear Michael:

I have reviewed the final version of the minutes of the Directorate for Mathematical and Physical Sciences Advisory Committee meeting that was held on April 22-23, 2004 (attached), and am pleased to certify the accuracy of these minutes. I appreciate the efforts of Morris Aizenman and other staff within MPS in getting these minutes prepared and in accommodating changes suggested by the Advisory Committee.

With best wishes,

Sincerely,

Jeanne E. Pemberton

Chair, MPS Advisory Committee

xc: M. Aizenman